

EAST Search History

Ref #	Hits	Search Query	DBs	Default Operator	Plurals	Time Stamp
L1	3	((("2882323") or ("5872277") or ("6278016"))).PN.	US-PGPUB; USPAT	OR	OFF	2007/05/30 12:48
L2	1	DE-3021414-\$.did.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2007/05/30 12:49
L3	2	DE-3105399-\$.did.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2007/05/30 12:51
L4	1	GB-1341015-\$.did.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2007/05/30 12:51
L5	2	GB-2051067-\$.did.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2007/05/30 12:52
L6	2	JP-60239443-\$.did.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2007/05/30 12:52
L7	0	WO-2000026175-\$.did.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2007/05/30 12:53
L8	1	WO-200026175-\$.did.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2007/05/30 12:54
L9	1105	diene near3 carboxylic adj acid	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2007/05/30 12:54
L10	454	I9 and @ad<="20030711"	US-PGPUB; USPAT; USOCR	OR	ON	2007/05/30 12:55
L11	363	myrcene near5 isoprene	US-PGPUB; USPAT; USOCR	OR	ON	2007/05/30 12:56
L12	257	I11 and @ad<="20030711"	US-PGPUB; USPAT; USOCR	OR	ON	2007/05/30 12:56

EAST Search History

L13	399	myrcene near5 isoprene	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	ON	2007/05/30 12:56
L14	257	l13 and @ad<="20030711"	US-PGPUB; USPAT; USOCR	OR	ON	2007/05/30 13:07
L15	0	l10 and l14	US-PGPUB; USPAT; USOCR	OR	ON	2007/05/30 13:03
L16	18353	"alkanoic acids"	US-PGPUB; USPAT; USOCR	OR	ON	2007/05/30 13:06
L17	605	"alkanoic acids".ti.	US-PGPUB; USPAT; USOCR	OR	ON	2007/05/30 13:08
L18	268	l17 and @ad<="20030711"	US-PGPUB; USPAT; USOCR	OR	ON	2007/05/30 13:08
L19	0	l14 and l18	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	ON	2007/05/30 13:07
L20	2636	"alkanoic acids".ti.	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	ON	2007/05/30 13:08
L21	268	l20 and @ad<="20030711"	US-PGPUB; USPAT; USOCR	OR	ON	2007/05/30 13:09
L22	1	l21 and myrcene	US-PGPUB; USPAT; USOCR	OR	ON	2007/05/30 13:09
L23	109	ester near5 diene adj compound	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	ON	2007/05/30 13:09
L24	67	l23 and @ad<="20030711"	US-PGPUB; USPAT; USOCR	OR	ON	2007/05/30 13:10
S1	239	"560/249".CCLS.	US-PGPUB; USPAT; USOCR	OR	ON	2007/05/30 10:30

EAST Search History

S2	21	((JAMES) near2 (BABLER)).INV.	US-PGPUB; USPAT; USOCR	OR	ON	2007/05/29 14:58
S3	3	((JAMES) near2 (BABLER)).INV.	EPO; JPO; DERWENT	OR	ON	2007/05/29 14:58
S4	239	"560/249".CCLS.	US-PGPUB; USPAT; USOCR	OR	ON	2007/05/29 15:01
S5	61	S4 and @ad<="20030711"	US-PGPUB; USPAT; USOCR	OR	ON	2007/05/30 12:55
S6	1	("5872277").PN.	US-PGPUB; USPAT	OR	OFF	2007/05/30 10:30
S7	1	("5872277").URPN.	USPAT	OR	ON	2007/05/30 11:44
S8	0	GB-1172516-\$.did.	USPAT	OR	ON	2007/05/30 11:45
S9	0	GB-1172516-\$.did.	US-PGPUB; USPAT; USOCR; EPO	OR	ON	2007/05/30 12:47

SEARCH HISTORY

=> d his nofile

(FILE 'HOME' ENTERED AT 10:23:49 ON 16 MAY 2007)

FILE 'HCAPLUS' ENTERED AT 10:24:09 ON 16 MAY 2007

E US20070055076/PN

L1 1 SEA ABB=ON PLU=ON US20070055076/PN
D ALL
SEL RN

FILE 'REGISTRY' ENTERED AT 10:25:28 ON 16 MAY 2007

L2 35 SEA ABB=ON PLU=ON (100-66-3/BI OR 105-87-3/BI OR
105-90-8/BI OR 105-91-9/BI OR 106-24-1/BI OR 106-25-2/B
I OR 106-42-3/BI OR 107-92-6/BI OR 108-21-4/BI OR
108-88-3/BI OR 108-90-7/BI OR 108-94-1/BI OR 109-20-6/B
I OR 1191-16-8/BI OR 123-35-3/BI OR 123-86-4/BI OR
127-08-2/BI OR 127-09-3/BI OR 137-40-6/BI OR 138-86-3/B
I OR 141-12-8/BI OR 142-96-1/BI OR 157258-67-8/BI OR
19559-59-2/BI OR 3915-83-1/BI OR 503-74-2/BI OR
5392-40-5/BI OR 556-82-1/BI OR 64-19-7/BI OR 78-79-5/BI
OR 78-93-3/BI OR 79-09-4/BI OR 79-31-2/BI OR 80-26-2/B
I OR 851785-97-2/BI)

L3 19 SEA ABB=ON PLU=ON L2 AND ?ACID?/CNS
D SCAN

L4 1 SEA ABB=ON PLU=ON 123-35-3/RN
D SCAN
D IDE

L5 1 SEA ABB=ON PLU=ON 78-79-5/RN
D SCAN
D IDE

L6 1 SEA ABB=ON PLU=ON 1191-16-8/RN
D SCAN
D CN
D IDE

L7 1 SEA ABB=ON PLU=ON 105-87-3/RN
D SCAN
D IDE

L8 1 SEA ABB=ON PLU=ON 141-12-8/RN
D IDE

L9 11 SEA ABB=ON PLU=ON L2 AND ?ACETATE?/CNS

FILE 'STNGUIDE' ENTERED AT 10:44:21 ON 16 MAY 2007

FILE 'CASREACT' ENTERED AT 10:50:09 ON 16 MAY 2007

L10 1 SEA ABB=ON PLU=ON 123-35-3/RCT(L) (105-87-3/PRO OR
141-12-8/PRO)
D SCAN

L11 2 SEA ABB=ON PLU=ON 78-79-5/RCT(L) 1191-16-8/PRO
D SCAN
E ESTER/CT
E ESTERS/CT

L12 23 SEA ABB=ON PLU=ON 64-19-7/RCT(L) (123-35-3/RCT OR
78-79-5/RCT)
D SCAN

L13 STR 123-35-3

L14 36 SEA SSS SAM L13 (448 REACTIONS)

L15 789 SEA SSS FUL L13 (11229 REACTIONS)
SAV L15 LAO307CRCT/A
E ESTERS/CT

L16 7147 SEA ABB=ON PLU=ON ESTERS+PFT, OLD, NT/CT

L17 7 SEA ABB=ON PLU=ON L15 AND L16
D SCAN
D SCAN
D QUE

SAV L17 LAO307CRCTA/A
 L18 STR L13
 L19 6 SEA SUB=L15 SSS SAM L18 (28 REACTIONS)
 D SCAN
 L20 88 SEA SUB=L15 SSS FUL L18 (708 REACTIONS)
 SAV L20 LAO307CRCTB/A
 L21 STR L18
 L22 1 SEA SUB=L15 SSS SAM L21 (7 REACTIONS)
 D SCAN
 L23 5 SEA SUB=L15 SSS FUL L21 (16 REACTIONS)
 D SCAN
 SAV L23 LAO307CRCTC/A
 L24 STR L21
 L25 1 SEA SUB=L15 SSS SAM L24 (7 REACTIONS)
 D SCAN
 L26 7 SEA SUB=L15 SSS FUL L24 (38 REACTIONS)
 D SCAN
 SAV L26 LAO307CRCTD/A
 SAV L27 LAO307CRCTE/A
 L27 34 SEA ABB=ON PLU=ON (L10 OR L11 OR L12) OR L17 OR L23
 OR L26
 L28 43 SEA ABB=ON PLU=ON BABLER JAMES?/AU
 L29 3 SEA ABB=ON PLU=ON L27 AND L28
 SAV L29 LAO307CRCTIN/A
 L30 31 SEA ABB=ON PLU=ON L27 NOT L29

FILE 'HCAPLUS' ENTERED AT 12:06:06 ON 16 MAY 2007

L31 QUE ABB=ON PLU=ON PY<2004 OR PRY<2004 OR AY<2004 OR
 MY<2004 OR REVIEW/DT
 L32 1 SEA ABB=ON PLU=ON L1 AND L31
 D SCAN

FILE 'CASREACT' ENTERED AT 12:07:53 ON 16 MAY 2007

L33 25 SEA ABB=ON PLU=ON L30 AND L31
 L34 3 SEA ABB=ON PLU=ON L29 AND L31

FILE 'HCAPLUS' ENTERED AT 12:08:48 ON 16 MAY 2007

D SCAN L1
 L35 619 SEA ABB=ON PLU=ON L4/RACT
 L36 5537 SEA ABB=ON PLU=ON L5/RACT
 L37 86 SEA ABB=ON PLU=ON L6/P
 L38 347 SEA ABB=ON PLU=ON L7/P
 D 1-2 KWIC
 L39 144 SEA ABB=ON PLU=ON L8/P
 D KWIC
 D 1-2 L36 KWIC
 L40 0 SEA ABB=ON PLU=ON L36(L) L37
 L41 12 SEA ABB=ON PLU=ON L36 AND L37
 L42 0 SEA ABB=ON PLU=ON L35(L) (L38 OR L39)
 L43 10 SEA ABB=ON PLU=ON L35 AND (L38 OR L39)
 L44 20 SEA ABB=ON PLU=ON (L40 OR L41 OR L42 OR L43)
 L45 34845 SEA ABB=ON PLU=ON L9
 L46 70 SEA ABB=ON PLU=ON (L35 OR L36) AND L45
 L47 4036 SEA ABB=ON PLU=ON L9/RACT
 L48 50 SEA ABB=ON PLU=ON (L35 OR L36) AND L47
 L49 9 SEA ABB=ON PLU=ON L48 AND L44
 E ESTERS/CT
 L50 QUE ABB=ON PLU=ON ESTERS+PFT,OLD,NT1/CT
 L51 70 SEA ABB=ON PLU=ON L44 OR L46 OR (L48 OR L49)
 L52 47 SEA ABB=ON PLU=ON L51 AND L50
 E VITAMINS/CT
 L53 QUE ABB=ON PLU=ON VITAMINS+PFT,OLD,NT/CT
 E FLAVOR/CT
 E FLAVORS/CT
 E FLAVORING/CT
 L54 QUE ABB=ON PLU=ON FLAVOR+PFT,OLD,NT/CT

L55 3 SEA ABB=ON PLU=ON L51 AND (L53 OR L54)
D SCAN
D SCAN L1
E "DIETARY SUPPLEMENTS"/CT
L56 QUE ABB=ON PLU=ON "DIETARY SUPPLEMENTS"+PFT,OLD,NT/CT
L57 QUE ABB=ON PLU=ON "FLAVORING MATERIALS"+PFT,OLD,NT/CT
L58 QUE ABB=ON PLU=ON "ODOR AND ODOROUS SUBSTANCES"+PFT,O
LD,NT/CT
L59 45 SEA ABB=ON PLU=ON L52 AND L31
SAV L59 LAO307HCP/A
L60 43 SEA ABB=ON PLU=ON L28
D QUE
L61 43 SEA ABB=ON PLU=ON L60 AND L31
L62 QUE ABB=ON PLU=ON VITAM? OR ODOR? OR SMELL? OR
PERFUM? OR SUPPLEMENT? OR FLAVOR?
L63 4 SEA ABB=ON PLU=ON L61 AND L62
L64 4 SEA ABB=ON PLU=ON L61 AND (L53 OR L56 OR L57 OR L58)
D QUE
L65 5 SEA ABB=ON PLU=ON L51 AND (L53 OR L56 OR L57 OR L58)
L66 45 SEA ABB=ON PLU=ON L55 OR L59 OR L65
L67 45 SEA ABB=ON PLU=ON L66 AND L31
SAV L67 LAO307HCP/A
L68 6 SEA ABB=ON PLU=ON L63 OR L64
L69 13 SEA ABB=ON PLU=ON L61 AND L50
L70 17 SEA ABB=ON PLU=ON L68 OR L69
SAV L70 LAO307HCPIN/A
D QUE L67
L71 43 SEA ABB=ON PLU=ON L67 NOT L70
D QUE L34
D QUE L33

FILE 'CASREACT' ENTERED AT 12:45:36 ON 16 MAY 2007
D QUE L33

FILE 'STNGUIDE' ENTERED AT 12:46:03 ON 16 MAY 2007

FILE 'MEDLINE, BIOSIS, DRUGU, EMBASE' ENTERED AT 12:46:36 ON 16
MAY 2007

L72 4 SEA ABB=ON PLU=ON L28
D 1-4 TI
SAV L72 LAO307IN/A

FILE 'STNGUIDE' ENTERED AT 12:47:53 ON 16 MAY 2007
D QUE L34
D QUE L70
D QUE L72

FILE 'CASREACT, HCAPLUS, BIOSIS' ENTERED AT 12:49:46 ON 16 MAY
2007

L73 19 DUP REM L34 L70 L72 (5 DUPLICATES REMOVED)
ANSWERS '1-3' FROM FILE CASREACT
ANSWERS '4-18' FROM FILE HCAPLUS
ANSWER '19' FROM FILE BIOSIS

FILE 'CASREACT' ENTERED AT 12:51:20 ON 16 MAY 2007

FILE 'CASREACT, HCAPLUS, BIOSIS' ENTERED AT 12:57:01 ON 16 MAY
2007

D L73 1-19 IBIB ABS

FILE 'CASREACT' ENTERED AT 12:57:02 ON 16 MAY 2007

FILE 'REGISTRY' ENTERED AT 12:57:42 ON 16 MAY 2007

D L4 IDE
D L5 IDE
D L6 IDE
D L7 IDE
D L8 IDE

FILE 'STNGUIDE' ENTERED AT 12:59:34 ON 16 MAY 2007

D QUE STAT L33
D QUE STAT L71

FILE 'CASREACT, HCAPLUS' ENTERED AT 13:00:44 ON 16 MAY 2007

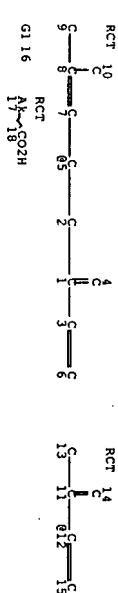
L74 67 DUP REM L33 L71 (1 DUPLICATE REMOVED)
ANSWERS '1-25' FROM FILE CASREACT
ANSWERS '26-67' FROM FILE HCAPLUS
D L74 1-25 IBIB ABS FHIT
D L74 26-67 IBIB ED ABS HITSTR HITIND

=> d his 134

L14 (FILE 'CASREACT' ENTERED AT 12:07:53 ON 16 MAY 2007)
 3 S L29 AND L31

=> d que 134

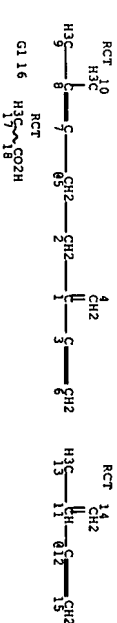
L10 1 SEA FILE-CASREACT ABB-ON PU-ON 123-35-3/RCT(L) (105-8
 7-3/PRO OR 141-12-8/PRO)
 L11 2 SEA FILE-CASREACT ABB-ON PU-ON 78-79-5/RCT(L) (1191-16
 -8/PRO)
 L12 23 SEA FILE-CASREACT ABB-ON PU-ON 64-19-7/RCT(L) (123-35
 -3/RCT OR 78-79-5/RCT)
 L13 STR



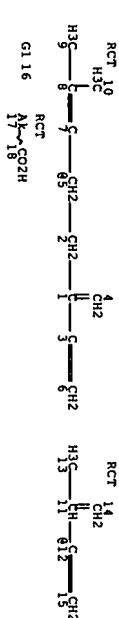
VAR G1=5/12
 NODE ATTRIBUTES:
 DEFAULT MLEVEL IS ATOM
 DEFAULT ELEVEL IS LIMITED
 ECOUNT IS M1-X7 C AT 17

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 18

STEREO ATTRIBUTES: NONE
 L15 789 SEA FILE-CASREACT SSS FUL L13 (11229 REACTIONS)
 L16 7147 SEA FILE-CASREACT ABB-ON PU-ON ESTERS+PFT, OLD, NT/CT
 L17 7 SEA FILE-CASREACT ABB-ON PU-ON L15 AND L16
 L21 STR



VAR G1=5/12
 NODE ATTRIBUTES:
 DEFAULT MLEVEL IS ATOM
 MLEVEL IS CLASS AT 2 4 5 6 9 10 11 13 14 15 17
 DEFAULT ELEVEL IS LIMITED
 GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 18
 STEREO ATTRIBUTES: NONE



VAR G1=5/12
 NODE ATTRIBUTES:
 CONNECT IS E1 RC AT 17
 DEFAULT MLEVEL IS ATOM
 MLEVEL IS CLASS AT 2 4 5 6 9 10 11 13 14 15
 DEFAULT ELEVEL IS LIMITED
 ECOUNT IS M1-X7 C AT 17

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 18

STEREO ATTRIBUTES: NONE
 L26 7 SEA FILE-CASREACT SUB-L15 SSS FUL L24 (38 REACTIONS
)
 L27 34 SEA FILE-CASREACT ABB-ON PU-ON (L10 OR L11 OR L12)
 OR L17 OR L21 OR L26
 L28 43 SEA FILE-CASREACT ABB-ON PU-ON BABLER JAMES7/AN
 L29 3 SEA FILE-CASREACT ABB-ON PU-ON L27 AND L28
 L31 QUE ABB-ON PU-ON FTY<2004 OR FTY<2004 OR AY<2004 OR
 M1<2004 OR REVIEW/DT
 L34 3 SEA FILE-CASREACT ABB-ON PU-ON L29 AND L31

=> d his 170

(FILE 'HCAPIUS' ENTERED AT 12:08:48 ON 16 MAY 2007)
 L70 17 S L68 OR L69

=> d que 170
 L28 43 SEA FILE-CASREACT ABB-ON PU-ON BABLER JAMES7/AN
 L31 QUE ABB-ON PU-ON FTY<2004 OR FTY<2004 OR AY<2004 OR
 M1<2004 OR REVIEW/DT
 L50 QUE ABB-ON PU-ON ESTERS+PFT, OLD, NT/CT
 L53 QUE ABB-ON PU-ON VITAMINS+PFT, OLD, NT/CT
 L56 QUE ABB-ON PU-ON DIETARY SUPPLEMENTS+PFT, OLD, NT/C
 L57 QUE ABB-ON PU-ON *FLAVORING MATERIALS+PFT, OLD, NT/C
 L58 QUE ABB-ON PU-ON *ODOR AND ODOROUS SUBSTANCES+PFT,
 OLD, NT/CT
 L60 43 SEA FILE-HCAPIUS ABB-ON PU-ON L28
 L61 43 SEA FILE-HCAPIUS ABB-ON PU-ON L60 AND L31
 L62 QUE ABB-ON PU-ON VITAM? OR ODO? OR SHEL? OR PERU
 M? OR SUPPLEMENT? OR FLAVOR?
 L63 4 SEA FILE-HCAPIUS ABB-ON PU-ON L61 AND L62
 L64 4 SEA FILE-HCAPIUS ABB-ON PU-ON L61 AND L56
 L68 6 SEA FILE-HCAPIUS ABB-ON PU-ON L63 OR L64
 L69 13 SEA FILE-HCAPIUS ABB-ON PU-ON L61 AND L50
 L70 17 SEA FILE-HCAPIUS ABB-ON PU-ON L68 OR L69

=> d his 172
(FILE 'MEDLINE, BIOSIS, DRUG, EMBASE' ENTERED AT 12:46:36 ON 16 MAY 2007)
L72 4 S L28
SAV L72 LA0307IN/A

FILE 'STINGUIDE' ENTERED AT 12:47:53 ON 16 MAY 2007

=> d que 172 43 SEA FILE-CASREACT ABB-ON PLU-ON BABLER JAMES7/AU
L72 4 SEA L28

=> dup rem 134 170 172
FILE 'CASREACT' ENTERED AT 12:49:46 ON 16 MAY 2007
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
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FILE 'HCAPLUS' ENTERED AT 12:49:46 ON 16 MAY 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)

FILE 'BIOSIS' ENTERED AT 12:49:46 ON 16 MAY 2007
COPYRIGHT (C) 2007 The Thomson Corporation
PROCESSING COMPLETED FOR L34
PROCESSING COMPLETED FOR L70
PROCESSING COMPLETED FOR L72

19 DUP REM 134 170 172 (5 DUPLICATES REMOVED)
ANSWERS '1-3' FROM FILE CASREACT
ANSWERS '4-18' FROM FILE HCAPLUS
ANSWER '19' FROM FILE BIOSIS

INVENTOR SEARCH RESULTS

=> d l73 1-19 1bib abs
YOU HAVE REQUESTED DATA FROM FILE 'CASREACT, HCAPLUS, BIOSIS' - CONTINUE
? (Y)/N:Y

L73 ANSWER 1 OF 19 CASREACT COPYRIGHT 2007 ACS ON STN DUPLICATE 1
ACCESSION NUMBER: 142:463897 CASREACT FULL-text
TITLE: Processes for synthesizing esters by 1,4-addition of alkanolic acids to myrcene or isoprene

INVENTOR(S): Babler, James H.
PATENT ASSIGNEE(S): Loyola University of Chicago, USA
SOURCE: PCT Int. Appl., 31 pp.
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
MO 2005044774	A1	20050519	MO 2004-0522075	20040708
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GR, GU, HT, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MY, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SN, SY, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
FW: BW, GH, GM, KE, LS, MM, MZ, NA, SD, SI, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, NG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GO, GW, ML, MR, NE, SN, TD, TG				
US 2007055076	A1	20070308	US 2006-564307	20061017
US 2003-486781P		20030711	MO 2004-0522075	20040708

PRIORITY APPLN. INFO.:
OTHER SOURCE(S): MARPAT 142:463897
AB A process was disclosed for synthesizing esters RCO2R1 (R = allyl; R1 = monoterpene moiety) which can be used in the manufacture of citral, precursors to citral and other products, such as vitamins, nutritional supplements, flavorings and fragrances. The process includes a 1,4-addition of an alkanolic acid to the conjugated diene of myrcene, which can be generated from β -pinene, or the conjugated diene of isoprene to produce esters thereof. Thus, myrcene was refluxed with AcONa/AcOH in Clph for 20 h to form a 70:30 mixture of geranyl acetate and neryl acetate in 60% yield.
REFERENCE COUNT: 4
THERE ARE 4 CITED REFERENCES AVAILABLE
FOR THIS RECORD. ALL CITATIONS AVAILABLE
IN THE RE FORMAT

L73 ANSWER 2 OF 19 CASREACT COPYRIGHT 2007 ACS ON STN DUPLICATE 2
ACCESSION NUMBER: 135:16653 CASREACT FULL-text
TITLE: Methods for conversion of isoprene to prenyl alcohol and esters
INVENTOR(S): Babler, James H.
PATENT ASSIGNEE(S): Loyola University of Chicago, USA
SOURCE: U.S., 7 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO. 6278016
 KIND B1
 DATE 20010821
 APPLICATION NO. US 1999-458153
 DATE 19991209
 PRIORITY APPL. INFO. US 1999-458153
 19991209
 OTHER SOURCE(S): MARPAT 135:16653
 AB Methods for preparing ester derivs. of 3-methyl-2-buten-1-ol (prenyl alc.) from the addition reaction of isoprene with alkanolic acids (e.g., acetic acid-acetic anhydride mixture) in the presence of an inorg. acid (e.g., phosphoric acid) catalyst are disclosed. The resultant prenyl ester (e.g., prenyl acetate) readily can be converted to prenyl alc. by saponification
 REFERENCE COUNT: 26
 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L73 ANSWER 3 OF 19 CASREACT COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 84:150125 CASREACT Full-text
 TITLE: A facile route to E-4-bromo-3-methyl-2-buten-1-ol. Application to the stereoselective synthesis of trisubstituted olefins
 AUTHOR(S): Babler, James H.; Butner, William J.
 CORPORATE SOURCE: Dep. Chem., Loyola Univ. Chicago, Chicago, IL, USA
 SOURCE: Tetrahedron Letters (1976), (4), 239-42
 CODEN: TETLEA; ISSN: 0040-4039

DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Addition of N-bromosuccinimide to isoprene in AcOH at 25° gave, after fractional distillation, 55% AcOCH₂CH:CHMeCH₂Br, which on hydrolysis and treatment with NaH gave (E)-ROCH₂CH:CHMeCH₂Br (1, R = H). Reaction of 1 (R = H, Ac) with Bu₂CuLi gave HOCH₂CH:CHMeCH₂Br and BuCH₂CH:CHMeCH₂Br, resp.

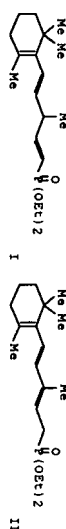
L73 ANSWER 4 OF 19 HCAPLUS COPYRIGHT 2007 ACS on STN DUPLICATE 3
 ACCESSION NUMBER: 2000:238081 HCAPLUS Full-text
 DOCUMENT NUMBER: 132:264887
 TITLE: Method of preparing 3-(3-methyl-2-buten-1-yl)-2,4-pentanedione and related dicarbonyl compounds
 INVENTOR(S): Babler, James H.; Posvic, Harvey W.
 PATENT ASSIGNEE(S): Loyola University of Chicago, USA
 SOURCE: U.S., 9 PP.
 DOCUMENT TYPE: Patent
 CODEN: USXXAM
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION: Patent

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6049010	A	20000411	US 1998-161983	1998 0929
			US 1998-161983	1998 0929

PRIORITY APPL. INFO.:
 OTHER SOURCE(S): CASREACT 132:264887; MARPAT 132:264887
 AB A method for preparation of a dicarbonyl compound by reacting a conjugated alkadiene compound with a 1,3-dicarbonyl compound in the presence of an acid catalyst is

described. E.g., polyphosphoric acid catalyzed the reaction of 2,4-pentanedione with isoprene to give 598-3-(3-methyl-2-buten-1-yl)-2,4-pentanedione.
 REFERENCE COUNT: 35
 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L73 ANSWER 5 OF 19 HCAPLUS COPYRIGHT 2007 ACS on STN DUPLICATE 4
 ACCESSION NUMBER: 1993:124810 HCAPLUS Full-text
 DOCUMENT NUMBER: 118:124810
 TITLE: An expedient route to a versatile intermediate for the stereoselective synthesis of all-trans-retinoic acid and beta-carotene
 AUTHOR(S): Babler, James H.; Schlidt, Scott A.
 CORPORATE SOURCE: Dep. Chem., Loyola Univ., Chicago, IL, 60626, USA
 SOURCE: Tetrahedron Letters (1992), 33(50), 7697-706
 CODEN: TETLEA; ISSN: 0040-4039
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 118:124810



AB Base-catalyzed isomerization of phosphonate I afforded the corresponding allylic phosphonate II as the sole product. Horner-Emmons olefination of Et trans-3-methyl-4-oxo-2-butenate with the ylide derived from II concludes a facile synthesis of the all-trans stereoisomer of Et retinoate.

L73 ANSWER 6 OF 19 HCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1998:621182 HCAPLUS Full-text
 DOCUMENT NUMBER: 129:230459
 TITLE: Methods for preparing prenyl alcohol
 INVENTOR(S): Babler, James H.
 PATENT ASSIGNEE(S): Loyola University of Chicago, USA
 SOURCE: PCT Int., 28 PP.
 DOCUMENT TYPE: Patent
 CODEN: PIXX02
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION: Patent

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9840345	A1	19980917	WO 1998-US256	1998 0108

W: AU, BR, CA, CN, ID, IL, JP, KP, KR, MX, AM, AZ, BY, KG,
 KZ, MD, RU, TJ, TM
 RM: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC,
 NL, PT, SE
 A 19990216 US 1997-814472
 US 5872277

CA 2281756 A1 19980917 CA 1998-2281756 <--
 1998
 0108

AU 9658171 A 19980929 AU 1998-58171 <--
 1998
 0108

EP 968170 A1 20000105 EP 1998-901716 <--
 1998
 0108

R: AT, BE, CH, DE, FR, GB, IT, LI, NL, SE
 JP 2001514652 T 20010911 JP 1998-539550 <--
 1998
 0108

PRIORITY APPL. INFO.:
 US 1997-814472 A <--
 1997
 0310

WO 1998-US256 W <--
 1998
 0108

OTHER SOURCE(S): CASREACT 129:230459; MARPAT 129:230459
 AB Methods for preparing 3-methyl-2-buten-1-ol (prenyl alc.) from 2-methyl-1,3-butadiene (isoprene) and carboxylic acids are disclosed. Carboxylic acids which can be used in the process have a K_{ow} relative to water greater than 10-4; dichloroacetic acid is especially preferred. The process involves the slow (e.g., dropwise) addition of isoprene to the carboxylic acid to form a prenyl ester. The ester-formation reaction proceeds at room temperature in most cases; use of an organic base catalyst, preferably a sodium or potassium salt of the reactant carboxylic acid, improves the yield. The resultant prenyl ester can be converted to prenyl alc. by reaction with a base. Prenyl alc. can be readily converted to citral, a chemical intermediate in the synthesis of vitamins A and E, and several widely-used carotenoids. Thus, isoprene was treated with dichloroacetic acid and sodium dichloroacetate at room temperature (with addns. of isoprene during the course of the reaction) to give 71% 3-methyl-2-butenyl dichloroacetate. This ester was further saponified to give 88% the expected 3-methyl-2-butenyl alc. Carrying out this experiment without the sodium dichloroacetate gave a product mixture containing only <50% the desired ester.

REFERENCE COUNT: 4
 THERE ARE 4 CITED REFERENCES AVAILABLE
 FOR THIS RECORD. ALL CITATIONS AVAILABLE
 IN THE RE FORMAT

L73 ANSWER 7 OF 19 HCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1996:1242785 HCAPLUS Full-text
 DOCUMENT NUMBER: 124:343745
 TITLE: A facile route to 3-alkoxy-3-methylpropenals, useful intermediates in the synthesis of carotenoids
 AUTHOR(S): Babelier, James H.; Lipcak, Vincent F.; Trautmann, Jeffrey A.; Zayia, Gregory H.
 CORPORA SOURCE: Dep. Chemistry, Loyola Univ., Chicago, Chicago, IL, 60626, USA
 SOURCE: Synthetic Communications (1996), 26(10), 1943-51
 CODEN: SYNCAV; ISSN: 0039-7911
 PUBLISHER: Dekker
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 124:343745
 AB A "one-pot" process for the preparation of a carotenoid synthon, EtOCH:CH=CHCHO, has been developed that involves methoxide-promoted condensation of propionaldehyde with Me

L73 ANSWER 8 OF 19 HCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1996:13322 HCAPLUS Full-text
 DOCUMENT NUMBER: 124:176588
 TITLE: Method of making 2,7-dimethyl-2,4,6-octatrienedial, a key intermediate in the commercial syntheses of various carotenoids
 INVENTOR(S): Babelier, James H.
 PATENT ASSIGNEE(S): Loyola University of Chicago, USA
 SOURCE: U.S., 9 pp.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5471005	A	19951128	US 1994-339659	1994 1118
WO 9616013	A1	19960530	WO 1995-US13372	1995 1011

W: AU, CA, JP, KP, KR
 RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE
 AU 9639601 A 19960617 AU 1995-39601
 1995
 1011

PRIORITY APPL. INFO.:
 US 1994-339659 A <--
 1994
 1118

WO 1995-US13372 W <--
 1995
 1011

OTHER SOURCE(S): CASREACT 124:176588
 AB A procedure for forming methylmalonaldehyde from propionaldehyde, an alkyl formate and a sodium alkoxide, utilizing a crossed-Claisen condensation is disclosed. The procedure avoids the formation of aldol condensation products. Also disclosed are processes for preparing 3-alkoxy-2-methylpropenals such as 2-methyl-3-(2-methyl-2-propenoxy)propenal from methylmalonaldehyde. The latter products are useful in the synthesis of carotenoids.

L73 ANSWER 9 OF 19 HCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1994:57133 HCAPLUS Full-text
 DOCUMENT NUMBER: 121:157133
 TITLE: Process for preparing 6,10,14-trimethyl-4-pentadecyn-6-ols
 INVENTOR(S): Babelier, James H.
 PATENT ASSIGNEE(S): Loyola University of Chicago, USA
 SOURCE: PCT Int. Appl., 57 pp.
 CODEN: PFXMDZ
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 16

SN 10/564307 Page 9 of 139 STIC STN SEARCH 5/17/2007

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9412457	A1	19940609	WO 1993-US10276	1993 1027
W: AU, CA, JP, KR, PT, SE RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL,				
JP 2002072251	A	20020312	JP 2001-160650	1991 0216
JP 2002100781	A	20020405	JP 2001-160671	1991 0216
JP 2003222838	A	20030808	JP 2002-331795	1991 0216
JP 3447730	B2	20030916	JP 2000-2212	1991 0327
JP 2000292813	A	20001020	JP 2000-121941	1991 0327
JP 2000330139	A	20001130	JP 2000-342919	1991 0327
JP 2001188257	A	20010710	JP 1998-38120	1991 0511
JP 10213819	A	19980811	JP 1998-323157	1991 0511
JP 11233791	A	19980827	JP 1999-153145	1992 0121
JP 2001144304	A	20010525	JP 1996-294546	1992 0124
JP 2000004024	A	20000107	JP 1992-59403	1992 0213
JP 3501977	B2	20040302		
JP 2000031498	A	20000128		
JP 09165791	A	19970624		
JP 05072564	A	19930326		

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SN 10/564307 Page 10 of 139 STIC STN SEARCH 5/17/2007

US 5218464

A

19930608

US 1992-836797

1992
0218

US 5349071	A	19940920	US 1992-976219	1992 1125
AU 9456644	A	19940622	AU 1994-56644	1993 1027
CN 1092758	A	19940928	CN 1993-120597	1993 1124
US 5410094	A	19950425	US 1994-255369	1994 0608
JP 08298331	A	19961112	JP 1996-95713	1996 0417
JP 2652366	B2	19970910	JP 1997-102689	1997 0404
JP 10041520	A	19980213	JP 1998-38121	1998 0204
JP 2890037	B2	19990510	JP 2001-142474	2001 0511
JP 10223910	A	19980821	JP 2003-168989	2003 0613
JP 3057049	B2	20000626	JP 2004-150976	2004 0520
JP 2002033332	A	20020131	JP 2004-150974	2004 0520
JP 3380546	B2	20030224	JP 1991-77318	1991 1125
JP 2004004890	A	20040108		
JP 3554563	B2	20040818		
JP 2004006950	A	20040108		
JP 2004258681	A	20040916		
JP 2004310123	A	20041104		
JP 2004334224	A	20041125		

PRIORITY APPLN. INFO.:

Page 10

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<--	JP 2000-13650	A3	0216
<--	JP 1997-215955	A3	0216
<--	JP 2000-2212	A3	0327
<--	JP 2000-342919	A3	0327
<--	JP 1995-335554	A3	0511
<--	JP 1998-38120	A3	0511
<--	JP 1998-38121	A3	0511
<--	JP 1998-124729	A3	0121
<--	JP 1999-153145	A3	0121
<--	JP 1992-34194	A3	0124
<--	JP 1992-38637	A3	0129
<--	JP 1992-187604	A3	0622
<--	WO 1993-US10276	W	1027
<--	JP 2001-92845	A3	0328

OTHER SOURCE(S): CASREACT 121:157133; MARPAT 121:157133
 AB Tertiary alkynols Me2CH(CH2)3CHMe(CH2)3C(OH)MeC(Tp)bond,CCCH2CH(OR)Me (R = H, alkyl, alkenyl, alkoxyalkyl, trialkylsilyl, arylalkyl) (e.g., 1-(1-octynyl)cyclohexanol).

L73 ANSWER 10 OF 19	HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER:	1991:649580 HCAPLUS Full-text
DOCUMENT NUMBER:	119:249580
TITLE:	Method of preparing C-18 ketones used in the preparation of vitamins E and K
INVENTOR(S):	Babier, James H.
PATENT ASSIGNEE(S):	Loyola University of Chicago, USA
SOURCE:	U.S., 13 pp.
DOCUMENT TYPE:	CODEN: USXXAM
LANGUAGE:	Patent
FAMILY ACC. NUM. COUNT:	English
PATENT INFORMATION:	1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5231232	A	19930727	US 1991-807462	1991
				1218

PRIORITY APPLN. INFO.: <--
 US 1991-807462 1991
 1218

OTHER SOURCE(S): CASREACT 119:249580
 AB Methods for preparing unsatd. C-18 ketones which can be used in the synthesis of vitamins E and K are claimed. One procedure involves coupling a C-9 primary allylic halide to a carbonyl-group-containing C-9 terminal alkene. A second, two-step procedure employs a C-4 bisallylic halide (molar excess) and a carbonyl-group-containing C-9 terminal alkene to form a C-13 primary allylic halide. The C-13 primary allylic halide can then be converted to the desired C-18 ketone by reaction with 2-methyl-3-buten-2-ol. Novel C-18 ketones (e.g., 14-hydroxy-6,14-dimethyl-10-methylene-5,10-pentadecene-7,12-diyne-2-one), C-13 allylic halides (e.g., 10-chloromethyl-6-methyl-5,10-undecadiene-7-yn-2-one) and C-9 allylic halides (e.g., 6-chloromethyl-2-methyl-6-hepten-3-yn-2-ol) are formed in the process.

L73 ANSWER 11 OF 19	HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER:	1992:490545 HCAPLUS Full-text
DOCUMENT NUMBER:	117:90545
TITLE:	Method of making 2,7-dimethyl-2,4,6-octatrienol and derivatives thereof
INVENTOR(S):	Babier, James H.
PATENT ASSIGNEE(S):	Loyola University of Chicago, USA
SOURCE:	U.S., 9 pp.
DOCUMENT TYPE:	CODEN: USXXAM
LANGUAGE:	Patent
FAMILY ACC. NUM. COUNT:	English
PATENT INFORMATION:	1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5107030	A	19920421	US 1991-661722	1991
				0304

WO 9215544	A1	19920917	WO 1992-US1462	1992
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W: AU, CA, JP, KR
 RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, MC, NL, SE
 AU 9215784 A 19921006 AD 1992-15784 1992 0225

PRIORITY APPL. INFO.:

US 1991-661722 A 1991 0304
 WO 1992-US1462 A 1992 0225

OTHER SOURCE(S):

CASREACT 117:90545; MARPAT 117:90545

AB The title compound (I) is prepared by treating RCH₂CH:CHCH₂R (R = Cl, Br) with >2 equivalent P(OR)₃ (R₁ = alkyl), treating (R₁O)₂CHCH:CHCH₂P(OR)₂ (II) with MeCOCH(OR)₂ (R₂ = alkyl; R₂ = alkylene) in the presence of >2 equivalent solid alkali metal hydride, and treating (R₂O)₂CHCH:CHCH:CHCH₂Cl (III) with aqueous acid in sep. steps. Thus, trans-ClCH₂CH:CHCH₂Cl was treated with P(OEt)₃ to give 87.5% II (R₁ = Et) which was treated with MeCOCH(OMe)₂ under phase-transfer conditions with KOH-PHMe-cyclohexane to give 71% III (R₂ = Me). Acetal hydrolysis with AcOH-aqueous THF gave 90% carotenoid intermediate I.

L73 ANSWER 12 OF 19 HCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1992:106507 HCAPLUS Full-text
 DOCUMENT NUMBER: 116:106507
 TITLE: Phosphonate reagent compositions and methods

INVENTOR(S): Babler, James H.
 PATENT ASSIGNEE(S): Loyola University of Chicago, USA
 SOURCE: Can. Pat. Appl., 33 pp.
 CODEN: CPXHEB

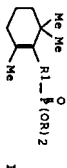
DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CA 2004125	A1	19910529	CA 1989-2004125	1989 1129

PRIORITY APPL. INFO.:

CA 1989-2004125

OTHER SOURCE(S): CASREACT 116:106507; MARPAT 116:106507



AB Novel phosphonate compds. of the formula I (R₁ = Me substituted pentadienyl, R = alkyl) are disclosed and claimed, as well as methods for manufacturing the phosphonates from C-14 through C-16 aldehydes. The phosphonate compds. of the present invention can be employed to form 13-cis-retinoic acid, retin-A and beta-carotene. E.g., a solution of 508 mg of methylenbisphosphonic acid tetra-Et ester (prepared from dibromomethane and tri-Et phosphite) in benzene was treated with NaH and then added to 208 mg of 2-methyl-4-(2,6,6-trimethyl-1-cyclohexenyl)-2-butenal, to give 93% yield of 3-methyl-5-(2,6,6-trimethyl-1-cyclohexenyl)-1,3-pentadienylphosphonic acid di-Et ester.

L73 ANSWER 13 OF 19 HCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1991:23509 HCAPLUS Full-text
 DOCUMENT NUMBER: 114:23509
 TITLE: Base-promoted rearrangement of carbonate esters derived from aldehyde cyanohydrins.

AUTHOR(S):

Babler, James H.; Marcuccilli, Charles J.;

CORPORATE SOURCE:

Oblong, John E.
 Dep. Chem., Loyola Univ. Chicago, Chicago, IL, 60626, USA

SOURCE:

Synthetic Communications (1990), 20(12), 1831-6

DOCUMENT TYPE:

CODEN: SYMCAV; ISSN: 0039-7911
 Journal

LANGUAGE:

English

OTHER SOURCE(S): CASREACT 114:23509
 AB Acylating HOCH₂CH(R = Ph, CH₂CHMe₂) with ClCO₂Et in pyridine gave 93-96% NCCROCO₂Et (I), which rearranged on treatment with LiN(SiMe₃)₂ in hexane-Et₂O-THF to give NCCROH(CO₂Et). These were cleaved with AgNO₃ and 2,6-lutidine in refluxing EtOH to give RCOCO₂Et in 50-86% overall yield from I.

L73 ANSWER 14 OF 19 HCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1988:186151 HCAPLUS Full-text
 DOCUMENT NUMBER: 108:186151
 TITLE: A facile route to α-amino acetals and the corresponding monoacetal derivatives of α-diketones with complete regiochemical control

AUTHOR(S): Babler, James H.; Marcuccilli, Charles J.
 CORPORATE SOURCE: Dep. Chem., Loyola Univ., Chicago, IL, 60626, USA

SOURCE:

Tetrahedron Letters (1987), 28(40), 4657-60

DOCUMENT TYPE:

CODEN: TELEAV; ISSN: 0040-4039
 Journal

LANGUAGE:

English

OTHER SOURCE(S): CASREACT 108:186151
 AB Treatment of RC(OEt)₃ (R = Et, Ph) with MeCOCH₂CH₂CO₂Et (I) in 65-80% yield, depending upon the conditions used to protonate the initial adduct, subsequent addition of R₁Li (R₁ = Me, Bu) or BuMgCl to I led to either RC(OEt)₂CH₂CH₂CO₂Et or RC(OEt)₂CH₂CO₂Et in >90% yield.

L73 ANSWER 15 OF 19 HCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1986:443114 HCAPLUS Full-text
 DOCUMENT NUMBER: 105:43114
 TITLE: Cyclopropanoid cyanooesters
 INVENTOR(S): Babler, James H.
 PATENT ASSIGNEE(S): Loyola University of Chicago, USA
 SOURCE: U.S., 10 pp.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1

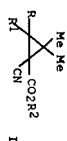
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4567265	A	19860128	US 1984-570874	1984 0116

PRIORITY APPLN. INFO.:

US 1984-570874	1984 0116
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OTHER SOURCE(S): CASREACT 105:43114; MARPAT 105:43114
GI



AB The title compds. (I; R = H, R1 = (halo)alkyl, (halo)alkenyl, cycloalkyl, cycloalkenyl, alkoxyalkenyl, naphthyl, furyl, thienyl, pyridinyl, pyrrolyl, indolyl, (un)substituted Ph; R1 = (CH2)n, CH2CH2CH2CH2; R2 = Me, Et; Z = O, S, MeN; n = 3-5), intermediates for pyrethroids, were prepared by cycloaddn. of R1C:(CN)CO2R2 with Me2CHNO2 in alc. solvents in presence of a base. Thus, NCCH2CO2Et and BzH were refluxed in HOAc containing β-alanine to give 92% (E)-PhCH:C(CN)CO2Et which was refluxed with Me2CHNO2 in EtOH containing NaOEt to give 96% I (R = H, R1 = Ph, Ph and CN cis).

L73 ANSWER 16 OF 19 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1985:203561 HCAPLUS Full-text
DOCUMENT NUMBER: 102:203561
TITLE: A facile method for the conversion of primary alkyl chlorides to the corresponding bromides
AUTHOR(S): Babler, James H.; Spina, Kenneth P.
CORPORATE SOURCE: Dep. Chem., Loyola Univ., Chicago, IL, 60626, USA
SOURCE: Synthetic Communications (1984), 14(14), 1313-19
CODEN: SYNCAV; ISSN: 0039-7911

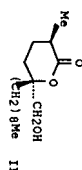
DOCUMENT TYPE: English
LANGUAGE: English
OTHER SOURCE(S): CASREACT 102:203561
AB The exchange reaction of RCH2Cl (R = 1-pentadecyl, MeCOCH2CH2CH2, 2-ClC6H4, CH2CH2CO2Et) with NaBr gave the resp. RCH2Br. 1-Chlorohexadecane was sited with NaBr, DMF, and CH2Br2 at 100° to give 1-bromohexadecane. Similarly, (ClCH2CH2)2O was converted to (BrCH2CH2)2O.

L73 ANSWER 17 OF 19 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1980:586089 HCAPLUS Full-text
DOCUMENT NUMBER: 93:186089
TITLE: Lactone formation via oxidative cyclization of an unsaturated carboxylic acid: application to the stereoselective synthesis of (+)-malynolide, an antibiotic from the marine blue-green alga Lyngbya majuscula
AUTHOR(S): Goment, Babler, James H.; Invergo, Benedict J.; Sarnesi, Steven J.

CORPORATE SOURCE:

Dep. Chem., Loyola Univ., Chicago, IL, 60626, USA

SOURCE: Journal of Organic Chemistry (1980), 45(21), 4241-3
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 93:186089
GI



AB Treatment of Me(CH2)8C:(CH2)1CH2CO2H (I) with 3-ClC6H4CO2H, followed by heating the intermediate epoxide in refluxing cyclohexane, afforded (+)-malynolide (II), a recently isolated marine natural product, in 50% yield. The olefinic acid I was in turn prepared in 5 steps from Me(CH2)8CHO, the key step involving a Michael reaction between MeCH(CO2Et)2 and 1-dodecen-3-one.

L73 ANSWER 18 OF 19 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1974:449207 HCAPLUS Full-text
DOCUMENT NUMBER: 81:49207
TITLE: Facile method for the bismethylation of ketones to functionalized trisubstituted olefins
AUTHOR(S): Babler, James H.; Olsen, Douglas O.
CORPORATE SOURCE: Dep. Chem., Loyola Univ., Chicago, IL, USA
SOURCE: Tetrahedron Letters (1974), (4), 351-4
CODEN: TELENY; ISSN: 0040-4039

DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 81:49207
AB R1C(OH)CH:CH2, prepared from R1CO(R = R1 = Ph; R, R1 = (CH2)5, R = Me, R1 = Ph, (CH2)4Me, CH:CH2), with AcOH-Ac2O gave 55-91% R1C:CHCH2OAc.

L73 ANSWER 19 OF 19 BIOSIS COPYRIGHT (c) 2007 The Thomson Corporation on STN
ACCESSION NUMBER: 1993:417023 BIOSIS Full-text
DOCUMENT NUMBER: PREV19934506468
TITLE: A facile route to allylic phosphonates via base-catalyzed isomerization of the corresponding vinyl phosphonates.
AUTHOR(S): Kiddle, James V.; Babler, James H. [Reprint author]
CORPORATE SOURCE: Dep. Chem., Loyola Univ., Chicago, IL, 60626, USA
SOURCE: Journal of Organic Chemistry, (1993) Vol. 58, No. 13, pp. 3572-3574.
CODEN: JOCEAH; ISSN: 0022-3263.
DOCUMENT TYPE: Article
LANGUAGE: English
ENTRY DATE: Entered STN: 15 Sep 1993
Last Updated on STN: 6 Nov 1993

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REGISTRY MOLECULES OF INTEREST

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(FILE 'REGISTRY' ENTERED AT 10:25:28 ON 16 MAY 2007)
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14 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2007 ACS ON STN
RN 123-35-3 REGISTRY
ED Entered STN: 16 Nov 1984

CN 1,6-octadiene, 7-methyl-3-methylene- (CA INDEX NAME)
OTHER NAMES:

β-octenolene

CN β-Myrcene

CN 2-Methyl-6-methylene-2,7-octadiene

CN 3-Methylene-7-methyl-1,6-octadiene

CN 7-Methyl-3-methylene-1,6-octadiene

CN Myrcene

CN NSC 406264

DR 2153-31-3

MF C10 H16

CI COM

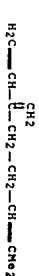
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STN Files: AGRICOLA, ANABSTR, BELISTEIN*, BIOSIS, BIOTECNO, CA, CAB, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMX, CHEMLIST, CIN, CSCHEM, CSNB, DDFU, DETHERM*, DRUGO, EMBASE, GHELIN*, HSDB*, IFCDB, IFIPAT, IFIUDB, IPA, MEDLINE, MRCK*, MSDS-OHS, NAPALERT, PIRA, PROMT, RTECS*, SPECINFO, SYNTLINE, TOXCENTER, ULIDAT, USPAT2, USPATFULL

(*File contains numerically searchable property data)

Other Sources: DSL**, EINECS**, TSCA**

(**Enter CHEMLIST file for up-to-date regulatory information)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

10169 REFERENCES IN FILE CA (1907 TO DATE)

51 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

10250 REFERENCES IN FILE CAPLUS (1907 TO DATE)

89 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> d his 15

(FILE 'REGISTRY' ENTERED AT 10:25:28 ON 16 MAY 2007)
1 S 78-79-5/RN

=> d 15 ide

15 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2007 ACS ON STN
RN 78-79-5 REGISTRY
ED Entered STN: 16 Nov 1984

CN 1,3-Butadiene, 2-methyl- (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Isoprene (8C1)

OTHER NAMES:

CN β-methylbiviny1

SN 10/564307 Page 18 of 139 STIC STN SEARCH 5/17/2007

CN 2-Methyl-1,3-butadiene
CN 2-Methylbutadiene
CN 3-Methyl-1,3-butadiene
CN Isoprenadiene
CN NSC 9237
DR 823271-95-0, 78006-92-5
MF C5 H8
CI COM

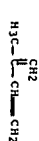
LC

STN Files: AGRICOLA, ANABSTR, AQUIRE, BELISTEIN*, BIOSIS, BIOTECNO, CA, CAOLD, CAPLUS, CASREACT, CSNB, CHEMCATS, CHEMINFORMX, CHEMLIST, CHEMSAFE, CIN, CSCHEM, CSNB, DETHERM*, EMBASE, ENCOMPAT, ENCOMPAT2, ENCOMPAT2, GHELIN*, HSDB*, IFCDB, IFIPAT, IFIUDB, IPA, MEDLINE, MRCK*, MSDS-OHS, NAPALERT, PIRA, PROMT, PS, RTECS*, SPECINFO, TOXCENTER, TUSA, ULIDAT, USPAT2, USPATFULL, VTB

(*File contains numerically searchable property data)

Other Sources: DSL**, EINECS**, TSCA**

(**Enter CHEMLIST file for up-to-date regulatory information)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

12878 REFERENCES IN FILE CA (1907 TO DATE)

596 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

12893 REFERENCES IN FILE CAPLUS (1907 TO DATE)

21 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> d his 16

(FILE 'REGISTRY' ENTERED AT 10:25:28 ON 16 MAY 2007)
1 S 1191-16-8/RN

=> d 16 ide

16 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2007 ACS ON STN
RN 1191-16-8 REGISTRY
ED Entered STN: 16 Nov 1984

CN 2-Buten-1-ol, 3-methyl-, 1-acetate (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 2-Buten-1-ol, 3-methyl-, acetate (6CI, 7CI, 8CI, 9CI)

OTHER NAMES:

CN 1,7-Dimethylallyl acetate

CN 1-Acetoxy-3-methyl-2-butene

CN 3,3-Dimethylallyl acetate

CN 3-Methyl-1-acetoxy-2-butene

CN 3-Methyl-2-buten-1-ol acetate

CN 3-Methyl-2-buten-1-yl acetate

CN Acetic acid 3-methyl-2-butenyl ester

CN Dimethylallyl acetate

CN Isopent-2-enyl acetate

CN Prenyl acetate

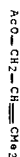
MF C7 H12 O2

CI COM

LC

STN Files: AGRICOLA, ANABSTR, BELISTEIN*, BIOSIS, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMX, CHEMLIST, CIN, CSCHEM, IFCDB, IFIPAT, IFIUDB, RTECS*, SPECINFO, TOXCENTER, USPAT2, USPATFULL

(*File contains numerically searchable property data)
Other Sources: DSL**, EINECS**, TSCA**
(**Enter CHEMIST file for up-to-date regulatory information)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

333 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
333 REFERENCES IN FILE CAPUS (1907 TO DATE)
8 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> d his 17

L7 (FILE 'REGISTRY' ENTERED AT 10:25:28 ON 16 MAY 2007)
1 S 105-87-3/RN

=> d 17 ide

L7 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2007 ACS on STN
RN 105-87-3 REGISTRY
ED Entered STN: 16 Nov 1984
CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2E)- (CA INDEX NAME)

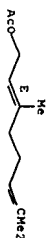
OTHER CA INDEX NAMES:
CN 2,6-Octadien-1-ol, 3,7-dimethyl-, acetate, (2E)- (9CI)
CN 2,6-Octadien-1-ol, 3,7-dimethyl-, acetate, (E)- (8CI)
CN Geraniol acetate (6CI)

OTHER NAMES:

CN (E)-3,7-Dimethyl-2,6-octadien-1-ol acetate
CN (E)-3,7-Dimethyl-2,6-octadienyl acetate
CN β-Geranyl acetate
CN Acetic acid geraniol ester
CN Bay pine (oyster) oil
CN Geranyl acetate
CN Geranyl ethanoate
CN NSC 2364
CN trans-1-Acetoxy-3,7-dimethyl-2,6-octadiene
CN trans-3,7-Dimethyl-2,6-octadien-1-yl acetate
CN trans-Geranyl acetate
FS STEREOSEARCH
DR 8022-83-1, 130396-84-8
MF C12 H20 O2
CI COM

LC STN Files: AGRICOLA, ANABSTR, BELLSTEIN, BIOSIS, BIOTECNO, CA, CAOLD, CAPUS, CASREACT, CANB, CHEMCATS, CHEMINFORMRX, CHEMIST, CINC, CSCHEM, DDFU, DETHERM, DRUGU, EMBASE, GHELIN, HSDR, IFCDB, IFIPAT, IFIUDB, IPA, MSDS-ONS, NAPRALENT, PROMT, RTECS, SPECINFO, TOXCENTER, USPAT2, USPATFUL
(*File contains numerically searchable property data)
Other Sources: DSL**, EINECS**, TSCA**
(**Enter CHEMIST file for up-to-date regulatory information)

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3624 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
3648 REFERENCES IN FILE CAPUS (1907 TO DATE)
63 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> d his 18

L8 (FILE 'REGISTRY' ENTERED AT 10:25:28 ON 16 MAY 2007)
1 S 141-12-8/RN

=> d 18 ide

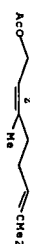
L8 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2007 ACS on STN
RN 141-12-8 REGISTRY
ED Entered STN: 16 Nov 1984
CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2Z)- (CA INDEX NAME)

OTHER CA INDEX NAMES:
CN 2,6-Octadien-1-ol, 3,7-dimethyl-, acetate, (2Z)- (9CI)
CN 2,6-Octadien-1-ol, 3,7-dimethyl-, acetate, (Z)- (8CI)
CN 2,6-Octadien-1-ol, 3,7-dimethyl-, formate, cis- (7CI)
CN Nerol acetate (6CI)

OTHER NAMES:

CN cis-1-Acetoxy-3,7-dimethyl-2,6-octadiene
CN cis-Geranyl acetate
CN Neryl acetate
CN STEREOSEARCH
DR 130396-85-9
MF C12 H20 O2
CI COM
SR CAS EARLY REGISTRATIONS
LC STN Files: AGRICOLA, ANABSTR, BELLSTEIN, BIOSIS, CA, CAOLD, CAPUS, CASREACT, CHEMCATS, CHEMINFORMRX, CHEMIST, CSCHEM, DDFU, DRUGU, GHELIN, IFCDB, IFIPAT, IFIUDB, NAPRALENT, RTECS, SPECINFO, TOXCENTER, USPAT2, USPATFUL
(*File contains numerically searchable property data)
Other Sources: DSL**, EINECS**, TSCA**
(**Enter CHEMIST file for up-to-date regulatory information)

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1605 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
1616 REFERENCES IN FILE CAPUS (1907 TO DATE)
27 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

STRUCTURE SEARCH

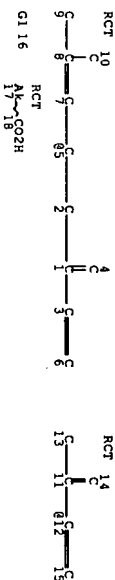
=> d his 133

(FILE 'HCAPIUS' ENTERED AT 12:06:06 ON 16 MAY 2007)

L13 FILE 'CASREACT' ENTERED AT 12:07:53 ON 16 MAY 2007
25 S L30 AND L31

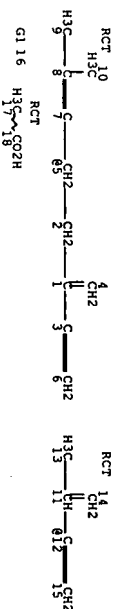
=> d que stat 133

L10 1 SEA FILE-CASREACT ABB-ON PUU-ON 123-35-3/RCT(L) (105-8
7-3/PRO OR 141-12-8/PRO)
L11 2 SEA FILE-CASREACT ABB-ON PUU-ON 78-79-5/RCT(L) (1191-16
-8/PRO)
L12 23 SEA FILE-CASREACT ABB-ON PUU-ON 64-19-17/RCT(L) (123-35
-3/RCT OR 78-79-5/RCT)
L13 STR



VAR G1-5/12
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED
ECCOUNT IS M1-X7 C AT 17
GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 18

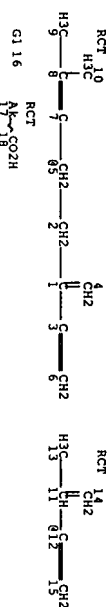
STEREO ATTRIBUTES: NONE
L15 789 SEA FILE-CASREACT SSS FUL L13 (11229 REACTIONS)
L16 7147 SEA FILE-CASREACT ABB-ON PUU-ON ESTERS+PTT,OLD,NT/CT
L17 7 SEA FILE-CASREACT ABB-ON PUU-ON L15 AND L16
L21 STR



VAR G1-5/12
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED
ECCOUNT IS M1-X7 C AT 17
GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 18

STEREO ATTRIBUTES: NONE

L23 5 SEA FILE-CASREACT SUB-L15 SSS FUL L21 (16 REACTIONS
L24 STR



VAR G1-5/12
NODE ATTRIBUTES:
CONNECT IS EL RC AT 17
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED
ECCOUNT IS M1-X7 C AT 17
GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 18

STEREO ATTRIBUTES: NONE
L26 7 SEA FILE-CASREACT SUB-L15 SSS FUL L24 (38 REACTIONS
L27 34 SEA FILE-CASREACT ABB-ON PUU-ON (L10 OR L11 OR L12)
OR L17 OR L23 OR L26
L28 43 SEA FILE-CASREACT ABB-ON PUU-ON BABLER JAMES7/AU
L29 3 SEA FILE-CASREACT ABB-ON PUU-ON L27 AND L28
L30 31 SEA FILE-CASREACT ABB-ON PUU-ON L27 NOT L29
L31 QUE ABB-ON PUU-ON PY<2004 OR PRY<2004 OR AY<2004 OR
MY<2004 OR REVIEW/DT
L33 25 SEA FILE-CASREACT ABB-ON PUU-ON L30 AND L31

=> d his 171

(FILE 'HCAPIUS' ENTERED AT 12:08:48 ON 16 MAY 2007)

L71 43 S L67 NOT L70

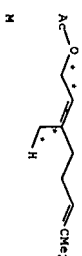
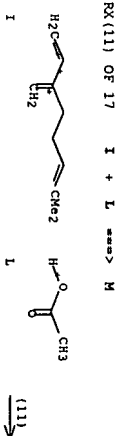
=> d que stat 171
L2 35 SEA FILE-REGISTRY ABB-ON PUU-ON (100-66-3/BI OR
105-87-3/BI OR 105-90-8/BI OR 105-91-9/BI OR 106-24-1/B
I OR 106-25-2/BI OR 106-42-3/BI OR 107-92-6/BI OR
108-21-4/BI OR 108-88-3/BI OR 108-90-7/BI OR 108-94-1/B
I OR 109-20-6/BI OR 1191-16-8/BI OR 123-35-3/BI OR
123-66-4/BI OR 127-08-2/BI OR 127-09-3/BI OR 137-40-6/B
I OR 138-86-3/BI OR 141-12-8/BI OR 142-96-1/BI OR
157256-67-8/BI OR 19559-59-2/BI OR 3915-83-1/BI OR
503-74-2/BI OR 5392-40-5/BI OR 556-82-1/BI OR 64-19-7/B
I OR 78-79-5/BI OR 78-93-3/BI OR 79-09-4/BI OR
79-31-2/BI OR 80-26-2/BI OR 831705-97-2/BI
L4 1 SEA FILE-REGISTRY ABB-ON PUU-ON 123-35-3/RN
L5 1 SEA FILE-REGISTRY ABB-ON PUU-ON 78-79-5/RN
L6 1 SEA FILE-REGISTRY ABB-ON PUU-ON 1191-16-8/RN
L7 1 SEA FILE-REGISTRY ABB-ON PUU-ON 105-87-3/RN
L8 1 SEA FILE-REGISTRY ABB-ON PUU-ON 141-12-8/RN
L9 11 SEA FILE-REGISTRY ABB-ON PUU-ON L2 AND FACETATE7/CNS

128 43 SEA FILE-CASREACT ABB-ON PLU-ON BABLER JAMES7/NU
 129 QUE ABB-ON PLU-ON PY<2004 OR PRY<2004 OR AY<2004 OR
 130 MY<2004 OR REVIEW/DT
 131 619 SEA FILE-HCAPLUS ABB-ON PLU-ON 14/RACCT
 132 5537 SEA FILE-HCAPLUS ABB-ON PLU-ON 15/RACCT
 133 86 SEA FILE-HCAPLUS ABB-ON PLU-ON 16/P
 134 347 SEA FILE-HCAPLUS ABB-ON PLU-ON 17/P
 135 144 SEA FILE-HCAPLUS ABB-ON PLU-ON 18/P
 136 0 SEA FILE-HCAPLUS ABB-ON PLU-ON 136(1),137
 137 12 SEA FILE-HCAPLUS ABB-ON PLU-ON 136 AND 137
 138 0 SEA FILE-HCAPLUS ABB-ON PLU-ON 135(1),138 OR 139
 139 10 SEA FILE-HCAPLUS ABB-ON PLU-ON 135 AND 138 OR 139
 140 20 SEA FILE-HCAPLUS ABB-ON PLU-ON 140 OR 141 OR 142 OR
 141 143
 142 34845 SEA FILE-HCAPLUS ABB-ON PLU-ON 19
 143 70 SEA FILE-HCAPLUS ABB-ON PLU-ON 135 OR 136 AND 145
 144 4036 SEA FILE-HCAPLUS ABB-ON PLU-ON 19/RACCT
 145 50 SEA FILE-HCAPLUS ABB-ON PLU-ON 135 OR 136 AND 147
 146 9 SEA FILE-HCAPLUS ABB-ON PLU-ON 148 AND 144
 147 0 SEA FILE-HCAPLUS ABB-ON PLU-ON 148 AND 144
 148 70 SEA FILE-HCAPLUS ABB-ON PLU-ON 144 OR 146 OR 148 OR
 149 149
 150 47 SEA FILE-HCAPLUS ABB-ON PLU-ON 151 AND 150
 151 0 SEA FILE-HCAPLUS ABB-ON PLU-ON 151 AND 150
 152 3 SEA FILE-HCAPLUS ABB-ON PLU-ON 151 AND 153 OR 154
 153 0 SEA FILE-HCAPLUS ABB-ON PLU-ON 151 AND 153 OR 154
 154 3 SEA FILE-HCAPLUS ABB-ON PLU-ON 151 AND 153 OR 154
 155 0 SEA FILE-HCAPLUS ABB-ON PLU-ON 151 AND 153 OR 154
 156 0 SEA FILE-HCAPLUS ABB-ON PLU-ON 151 AND 153 OR 154
 157 0 SEA FILE-HCAPLUS ABB-ON PLU-ON 151 AND 153 OR 154
 158 0 SEA FILE-HCAPLUS ABB-ON PLU-ON 151 AND 153 OR 154
 159 45 SEA FILE-HCAPLUS ABB-ON PLU-ON 152 AND 131
 160 43 SEA FILE-HCAPLUS ABB-ON PLU-ON 152 AND 131
 161 43 SEA FILE-HCAPLUS ABB-ON PLU-ON 152 AND 131
 162 0 SEA FILE-HCAPLUS ABB-ON PLU-ON 152 AND 131
 163 0 SEA FILE-HCAPLUS ABB-ON PLU-ON 152 AND 131
 164 4 SEA FILE-HCAPLUS ABB-ON PLU-ON 152 AND 131
 165 4 SEA FILE-HCAPLUS ABB-ON PLU-ON 152 AND 131
 166 5 SEA FILE-HCAPLUS ABB-ON PLU-ON 152 AND 131
 167 45 SEA FILE-HCAPLUS ABB-ON PLU-ON 152 AND 131
 168 6 SEA FILE-HCAPLUS ABB-ON PLU-ON 152 AND 131
 169 13 SEA FILE-HCAPLUS ABB-ON PLU-ON 152 AND 131
 170 17 SEA FILE-HCAPLUS ABB-ON PLU-ON 152 AND 131
 171 43 SEA FILE-HCAPLUS ABB-ON PLU-ON 152 AND 131

=> dup rem 133 171
 FILE 'CASREACT' ENTERED AT 13:00:44 ON 16 MAY 2007
 USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT.
 COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)
 FILE 'HCAPLUS' ENTERED AT 13:00:44 ON 16 MAY 2007
 USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT.
 PLEASE SEE "HELP USAGETEXTS" FOR DETAILS.
 COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)
 PROCESSING COMPLETED FOR 173
 67 DUP REM 133 171 (1 DUPLICATE REMOVED)
 ANSWERS '1-25' FROM FILE CASREACT
 ANSWERS '26-67' FROM FILE HCAPLUS

STRUCTURE SEARCH RESULTS

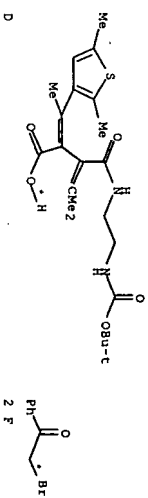
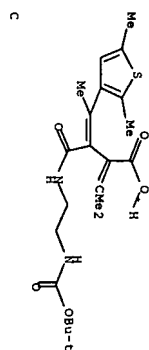
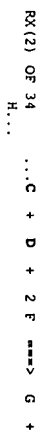
174 ANSWER 1 OF 67 CASREACT COPYRIGHT 2007 ACS ON STN DUPLICATE 1
 ACCESSION NUMBER: 116:6750 CASREACT FULL-TEXT
 TITLE: Hydrochlorination of myrcene. Selectivity for
 Cl.
 AUTHOR(S): De Doldan, Griselda V.; Cardelli, Daniel; De
 Schilluk, Irma G.
 CORPORATE SOURCE: Inst. Invest. Prod. Nat., IPNAYS, Santa Fe,
 3000, Argent.
 SOURCE: Essence, Derivati Agrumari (1990),
 60(3), 350-7
 CODEN: EDGAMH; ISSN: 0014-0902
 DOCUMENT TYPE: Journal
 LANGUAGE: Spanish
 AB Conditions favoring C(1)-chlorination in the hydrochlorination of β -myrcene were
 examined. The monochloro derivs. were hydrolyzed to the alcs. (geraniol, nerol, etc.),
 which are used in various aromas.



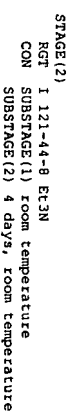
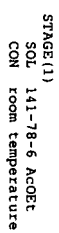
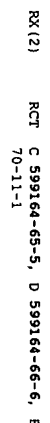
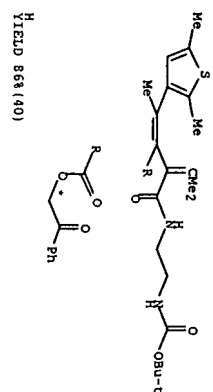
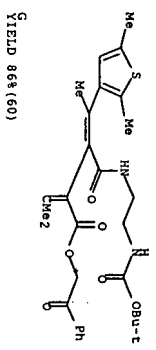
RX(11) RCT I 123-35-3, L 64-19-7
 RGT J 7647-01-0 HCL, D 75-44-5 COC12
 PRO M 16409-44-2

174 ANSWER 2 OF 67 CASREACT COPYRIGHT 2007 ACS ON STN
 ACCESSION NUMBER: 139:245608 CASREACT FULL-TEXT
 TITLE: Syntheses and UV/VIS properties of
 amino-functionalized polyimides
 AUTHOR(S): Otto, Bernadot; Rueck-Braun, Karola
 CORPORATE SOURCE: Institut fuer Chemie, Technische Universitaet
 Berlin, Fakultae II, TC 2, Berlin, 10623,
 Germany
 SOURCE: European Journal of Organic Chemistry (2003), (13), 2409-2417
 PUBLISHER: CODEN: EJOCHF; ISSN: 1434-193X
 DOCUMENT TYPE: Wiley-VCH Verlag GmbH & Co. KGaA
 LANGUAGE: Journal
 English

AB Functionalized fulgimides are regarded as a promising class of photochromic compds. for modulating the structure and function of biomols. A new synthetic route to fulgimides bearing amino-functionalized substituents at the imide N atom was developed. The synthesis of the fulgimides was achieved by base-catalyzed cyclization of phenacyl esters of the succinamic acids derived from fulgides and N-boc-protected alkyl- and aryl-substituted diamines with triethylamine or tert-butyl lithium. The UV/visible spectroscopic data and the photochromic properties of these new compds. were studied.

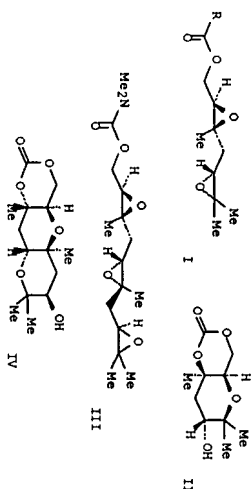


(2)



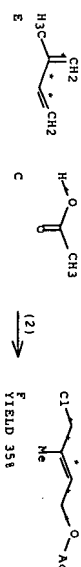
PRO G 599164-67-7, H 599164-68-8
REFERENCE COUNT: 40
THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L74 ANSWER 3 OF 67 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 139:117351 CASREACT FULL-TEXT
TITLE: Biomimetic Synthesis of Fused Polypyridines: Oxacyclization Stereo- and Regioselectivity Is a Function of the Nucleophile
AUTHOR(S): Bravo, Fernando; McDonald, Frank E.; Nelvert, Wade A.; Do, Bao; Haddad, Kenneth I.
CORPORATE SOURCE: Department of Chemistry, Emory University, Atlanta, GA, 30322, USA
SOURCE: Organic Letters (2003), 5(12), 2123-2126
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



AB The stereoselectivity of Lewis acid-induced endo-regioselective oxacyclizations of 1,4-diepoxydes is dependent upon the nature of the terminating nucleophile. For instance, ring-opening/recyclization of the carbonate-substituted diepoxide I (R = Me₃CO) provides a cis-fused bicyclic product II, whereas carbonate-derived I (R = Me₂N) affords the trans-fused diastereomer of II. Stereospecific and regioselective conversion of the tertiary carbonate-terminated 1,4,7-triepoxy III to tricyclic all-trans-fused polypyrans IV is also demonstrated.

RX(2) OF 111 E + C ==> F...



RX(2) RCT E 78-79-5, C 64-19-7

STAGE(1)

RGT B 507-40-4 t-Bu hypochlorite
SOL 64-19-7 AcOH
CON 1 hour, room temperature

STAGE(2)

RGT G 1310-73-2 NaOH
SOL 7732-18-5 Water

PRO F 24529-80-4

REFERENCE COUNT: 42 NTE stereoselective

THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L74 ANSWER 4 OF 67 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 141:350066 CASREACT FULL-TEXT
TITLE: Synthesis and characterization of new chromano isoxazoles

AUTHOR(S):

Randa, Rani; Rao, Palli. S.; Suryaprabha, R.;
Lakshmi, V. V.; Acharyulu, P. V. N.; Murthy,
Y. L. N.
Dept. of Organic Chemistry, Andhra University,
Visakhapatnam, India

SOURCE:

Chemistry (Rajkot, India) (2003),
1(4), 246-250

CODEN: CHEMCT; ISSN: 0972-8376

PUBLISHER: Trade Science Inc.
DOCUMENT TYPE: Journal

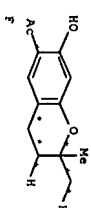
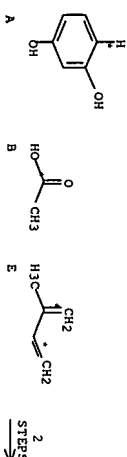
LANGUAGE:

English

AB The title compds., (five new chromano isoxazoles) were synthesized by condensation of chalcones with hydroxylamine hydrochloride in the presence of alic. KOH. The synthesis involves four steps- Starting with the acylation of Resorcinol using anhydrous ZnCl₂ and glacial acetic acid, which afforded Resacetophenone. Resacetophenone was then subjected to nuclear prenylation using isoprene in the presence of polyphosphoric acid and xylene, to form 7-hydroxy-6-acetyl 2,2'-dimethyl chroman. Condensation of Chroman with various substituted benzaldehydes in the presence of alic. KOH furnished different chalcones. Finally, Chalcones were condensed with hydroxylamine hydrochloride in alkaline KOH medium and the title compds. were obtained. Compds. thus obtained were characterized by various spectroscopic techniques to confirm their structures.

RX(13) OF 38 COMPOSED OF RX(1), RX(2)

RX(13) A + B + E ==> F



RX(1) RCT A 108-46-3, B 64-19-7

RGT D 7646-85-7 ZnCl₂

PRO C 89-84-9

SOL 64-19-7 AcOH

RX(2) RCT E 78-79-5, C 89-84-9

PRO F 31273-58-2

SOL 1330-20-7 Xylene

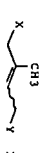
REFERENCE COUNT: 9 NTE Polyphosphoric acid used

THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L74 ANSWER 5 OF 67 CASREACT COPYRIGHT 2007 ACS on STN

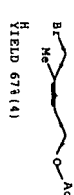
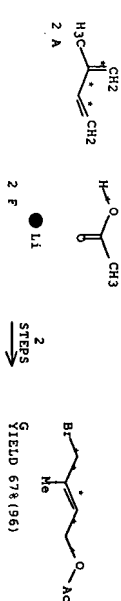
ACCESSION NUMBER: 137:140330 CASREACT Full-text
 TITLE: Process for producing allyl halide compounds
 INVENTOR(S): Doi, Noriyuki; Seko, Shinzo; Kimura, Kazutaka;
 Takahashi, Toshiya
 PATENT ASSIGNEE(S): Japan
 SOURCE: U.S. Pat. Appl. Publ., 8 pp.
 CODEN: USXACO
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002107422	A1	20020808	US 2002-62537	20020205
JP 2002241360	A	20020828	JP 2001-36572	20010214
EP 1231197	A1	20020814	EP 2002-2168	20020129
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, NO, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2003212825	A	20030730	JP 2002-27910	20020205
CN 1373112	A	20021009	CN 2002-107071	20020207
PRIORITY APPL. INFO.:			JP 2001-30670	20010207
			JP 2001-36572	20010214
			JP 2001-349769	20011115



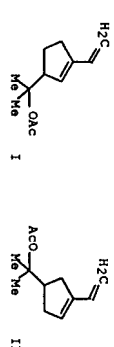
AB Comps. comprising (E)-1,4-dibromo-2-methyl-2-butene and (Z)-1,4-dibromo-2-methyl-2-butene are prepared where the ratio of the E isomer to the total amount of the E and Z isomers is 20:9; a process for producing these compts. and using them to produce an allyl halide compound [I; X = bromine; Y = ASO₂, RCO₂; A = (un)substituted aryl; R = H, lower alkyl, (un)substituted aryl; the wavy line means that the derivative is a mixture of an E or Z geometrical isomer; e.g., (E)-1-(phenylsulfonyl)-3-methyl-4-bromo-2-butene] is described.

RX (7) OF 11 COMPOSED OF RX (1), RX (2)
 RX (7) 2 A + 2 F ==> G + H



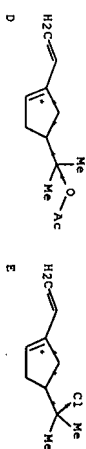
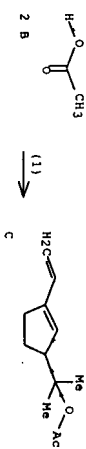
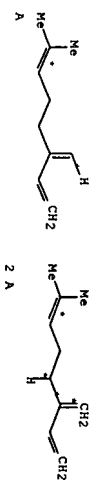
RX (1) RCT A 78-79-5
 RCT D 7726-95-6 B12
 PRO B 16526-19-5, C 16526-18-4
 SOL 25154-42-1 Butane, Chloro-
 RX (2) RCT B 16526-19-5, C 16526-18-4, F 546-89-4
 PRO G 32659-14-6, H 32659-13-5
 SOL 7732-18-5 Water, 68-12-2 DMF

L74 ANSWER 6 OF 67 CASREACT COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 137:295105 CASREACT Full-text
 TITLE: Palladium catalyzed oxidation of monoterpenes:
 novel oxidation of myrcene with dioxygen
 AUTHOR(S): Goncalves, Jose Alton; Howarth, Oliver W.;
 Gusvinskaya, Elena V.
 CORPORATE SOURCE: Departamento de Quimica, Universidade Federal
 de Minas Gerais, Belo Horizonte, MG,
 31270-901, Brazil
 SOURCE: Journal of Molecular Catalysis A: Chemical (2002), 185(1-2), 97-104
 CODEN: JMCCEZ; ISSN: 1381-1169
 PUBLISHER: Elsevier Science B.V.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB Myrcene can be efficiently and selectively oxidized by dioxgen in glacial acetic acid containing LiCl, in the presence of the PdCl₂-CuCl₂ catalytic combination, yielding two isomers of a new functionalized monoterpene, i.e., 3-(1-acetoxy-1-methylethyl)-1-vinylcyclopentene (I) and 4-(1-acetoxy-1-methylethyl)-1-vinylcyclopentene (II), as major products. These compts. have a pleasant scent with a flower or fruit tinge and could be used as components of synthetic perfumes. The activities of Pd(OAc)₂-LiNO₃, Pd(OAc)₂-Cu(NO₃)₂ and Pd(OAc)₂-benzoquinone systems in myrcene oxidation have also been examined

RX (1) OF 1 3 A + 2 B ==> C + D + E



RX(1) RCT A 123-35-3, B 64-19-7

PRO C 467449-32-7, D 467449-34-9, E 467449-33-8

CAT 7647-10-1 PdCl₂, 7447-39-4 CuCl₂

SOL 64-19-7 AcOH
REFERENCE COUNT: 27
THERE ARE 27 CITED REFERENCES AVAILABLE
FOR THIS RECORD. ALL CITATIONS AVAILABLE
IN THE RE FORMAT

L74 ANSWER 7 OF 67 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 136:150747 CASREACT FULL-TEXT

TITLE: Nickel-catalyzed homopolymerization of aldehydes

AUTHOR(S): Kimura, Masamichi; Ezoe, Akihito; Tanaka, Shuji; Tamate, Yoshino

CORPORATE SOURCE: Department of Applied Chemistry, Faculty of Engineering, Nagasaki University, Nagasaki, 852-8521, Japan

SOURCE: Angewandte Chemie, International Edition (2001), 40(19), 3600-3602

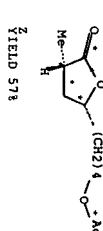
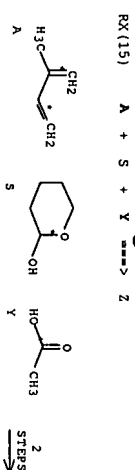
PUBLISHER: Wiley-VCH Verlag GmbH

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Aldehydes and cyclic hemiacetals were efficiently homopolymerized in presence of Ni(acac)₂ and Et₃B in THF. The reaction proceeded in reasonable yields with aqueous glutaraldehyde.

RX(15) OF 18 COMPOSED OF RX(7), RX(11)



RX(7) RCT A 78-79-5, S 694-54-2

RCT D 97-94-9 Et₃B

PRO T 394217-74-4

CAT 3264-82-2 Ni, acetylacetonate

SOL 109-99-9 THF, 110-54-3 Hexane

NTE stereoselective, regioselective

RX(11) RCT T 394217-74-4

STAGE(1) RCT AA 10028-15-6 Ozonide

SOL 75-09-2 CH₂Cl₂

STAGE(2) RCT Y 64-19-7

RCT AB 7722-84-1 H₂O₂

SOL 7664-93-9 H₂SO₄

SOL 64-19-7 AcOH, 7732-18-5 Water

PRO 2 394217-78-8

REFERENCE COUNT: 21

THERE ARE 21 CITED REFERENCES AVAILABLE
FOR THIS RECORD. ALL CITATIONS AVAILABLE
IN THE RE FORMAT

L74 ANSWER 8 OF 67 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 134:29587 CASREACT FULL-TEXT

TITLE: New Synthesis of the Alkaloid Poloniumtoxin C

AUTHOR(S): Van, T. N.; De Kimppe, N.

CORPORATE SOURCE: Faculty of Agricultural and Applied Biological Sciences, Department of Organic Chemistry, Ghent University, Ghent, B-9000, Belg.

SOURCE: Tetrahedron (2000), 56(40), 7965-7973

PUBLISHER: Elsevier Science Ltd.

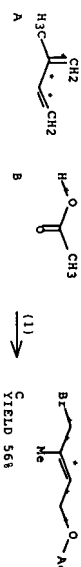
DOCUMENT TYPE: Journal

LANGUAGE: English

AB Two new short syntheses of the alkaloid poloniumtoxin C were presented. In the first pathway, poloniumtoxin C was obtained in two steps by alkylation of 6-methyl-2,3,4,5-tetrahydro-2-pyridine with (E)-4-bromo-3-methyl-1-(tetrahydro-2-pyran-2-yl)-2-butene and

subsequent deprotection of the THF group. In the second pathway, the cyclic ketimine was constructed via a short sequence of reactions involving first a sequential allylation of the N-(4-isopropylidene)isopropylamine with N,N-disilylprotected α-bromopropylamine and (E)-4-bromo-3-methyl-1-(tetrahydro-2-pyran-2-yl)-2-butene, then transamination and deprotection, with the latter two reactions occurring in one step.

RX (1) OF 28 A + B ==> C...



RX (1) RCT A 78-79-5, B 64-19-7

STAGE (1)

RGT D 128-08-5 Bromosuccinimide

SOL 64-19-7 AcOH

STAGE (2)

SOL 7732-18-5 Water

STAGE (3)

SOL 75-09-2 CH2Cl2

PRO C 32659-14-6

NTE STEREoselective

REFERENCE COUNT: 11

THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L74 ANSWER 9 OF 67 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 130:325271 CASREACT Full-text
Preparation of 8-ocimene] esters for use in perfumes and as aromatic substances

INVENTOR(S):

Sutburg, Horst; Sommer, Horst; Lambrecht, Stefan; Moerner, Peter; Guentert, Matthias; Kindel, Guentert; Koppe, Volkmar; Hartmann und Reimer G.m.b.H., Germany

PATENT ASSIGNEE(S):

Ger. Offen., 14 pp.

SOURCE:

CODEN: GXXBX

DOCUMENT TYPE:

Patent

LANGUAGE:

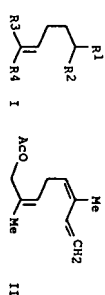
German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

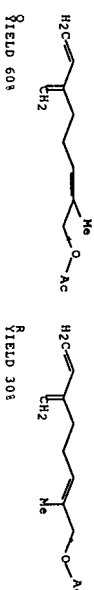
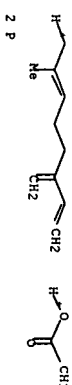
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19748774	A1	19990506	DE 1997-19748774	19971105
EP 915079	A1	19990512	EP 1998-120071	19981023
EP 915079	B1	20030806		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
ES 2207778	T3	20040601	ES 1998-120071	19981023
JP 1126330	A	19990831	JP 1998-324452	19981030
JP 3583933	B2	20041104		
US 6034268	A	20000307	US 1998-186267	19981104

PRIORITY APPL. INFO.: DE 1997-19748774 19971105
OTHER SOURCE(S): MARPAT 130:325271



AB Compds. I (R1, R2 = Me, vinyl; R3, R4 = Me, CH2O2CR5; R5 = H, C1-6-alkyl, C2-6-alkenyl) are useful as scents and aromatic substances. Thus, (32, 62)-II was prepared from (E/Z)-ocimene via chlorination with NaOCl solution followed by acetylation with NaOAc in DMF containing NaI. (32, 62)-II has a light fresh-green, fruity odor.

RX (4) OF 22 2 P + 2 B ==> Q + R...



RX (4) RCT P 123-35-3

STAGE (1)

RGT J 7681-52-9 NaOCl, K 64-19-7 AcOH

SOL 7732-18-5 Water

STAGE (2)

RCT B 127-09-3

RGT G 7681-82-5 NaI

SOL 68-12-2 DMF

PRO Q 38228-41-0, R 98666-05-8

L74 ANSWER 10 OF 67 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 129:343135 .CASREACT FULL-text
TITLE: Diastereoselective azidination of alkenes using 3-acetoxymino-2-(1-hydroxyalkyl)guinazolin-4(3H)-ones in the presence of titanium(IV) tert-butoxide P.; Atkinson, Robert S.; Ayrescough, Andrew P.; Gattrell, W. T.; Raynham, Tony M.; Dep. Chem., Univ. Leicester, LE1 7RH, UK Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1998), (17), 2783-2793 CODEN: JCPR84; ISSN: 0300-922X

AUTHOR(S):
CORPORATE SOURCE:
SOURCE:

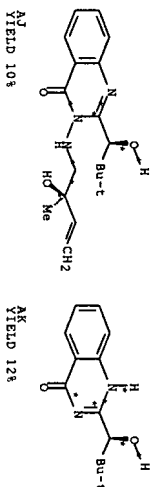
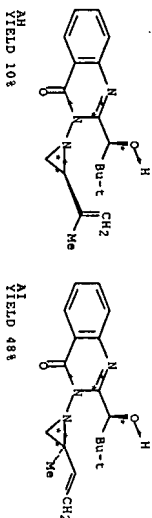
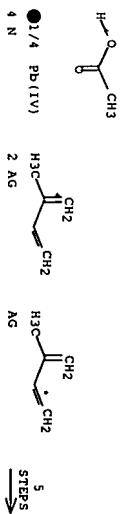
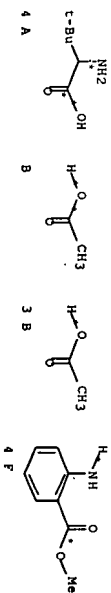
PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

AB 3-Amino-2-(1(S)-1-hydroxy-2,2-dimethylpropyl)guinazolin-4(3H)-one 9 (Q2NH) was prepared in four steps from (S)-tert-leucine in 43% yield without the need for chromatography. The corresponding 3-acetoxy-mino-guinazolinone, prepared in dichloromethane solution by reaction of 9 with lead tetraacetate, reacts with alkenes in the presence of titanium(IV) tert-butoxide to give the corresponding azidines stereoselectively. With styrene and butadiene the corresponding azidines were obtained completely stereoselectively. Indene gave the expected endo-N-invertomer of azidine as the kinetically-formed product (86%) also completely stereoselectively: equilibration to give a 8:1 ratio of exo:endo N-invertomers occurs above 0°C. From an X-ray structure determination one azidine product, the sense of diastereoselectivity in its formation is in agreement with the transition state model. Azidinations of Me acrylate and of tert-Bu acrylate give the resp. products highly stereoselectively (dr20:1) and with the same sense of diastereoselectivity as identified by an X-ray crystal structure determination previously. Azidinations of α-methylstyrene and Me methacrylate are less completely diastereoselective; isoprene reacts completely diastereoselectively at its unsubstituted double bond but with little diastereoselectivity at its methyl-substituted double bond and the regioselectivity of azidination on the two double bonds is 1.4:1 resp. by comparison to 1.4:7 in the absence of titanium(IV) tert-butoxide.

RX(108) OF 127 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(13)
RX(108) ==> AH + AI + AJ + AK



RX(1) RCT A 20859-02-3, B 64-19-7

STAGE(1)
RCT D 7631-99-4 NaNO3
SOL 64-19-7 AcOH

STAGE(2)
SOL 7732-18-5 Water

PRO C 84621-74-9
NTE STEREOSELECTIVE

RX(2) RCT C 84621-74-9

STAGE(1)
RCT H 68-12-2 DMF, I 7719-09-7 SOCl2
SOL 60-29-7 Et2O

STAGE(2)
RCT F 134-20-3

PRO G 215546-92-2
NTE STEREOSELECTIVE

RX(3) RCT G 215546-92-2

STAGE(1)
RCT L 302-01-2 N2H4
SOL 64-17-5 EtOH

STAGE(2)
SOL 7732-18-5 Water

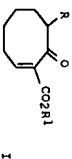
PRO K 182160-10-7
NTE STEREOSELECTIVE

RX (4) RCT K 182160-10-7, N 546-67-8
 PRO O 182160-08-3
 SOL 865-49-6 CDC13
 RTE STEREoselective

RX (13) RCT O 182160-08-3, AG 78-79-5
 PRO AH 215546-97-7, AI 215546-96-6, AJ 215546-98-8, AK
 215546-99-9
 SOL 75-09-2 CH2C12
 RTE STEREoselective

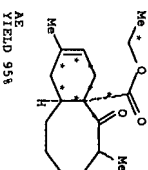
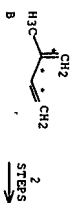
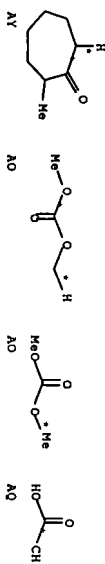
REFERENCE COUNT: 22
 THERE ARE 22 CITED REFERENCES AVAILABLE
 FOR THIS RECORD. ALL CITATIONS AVAILABLE
 IN THE RE FORMAT

L74 ANSWER 11 OF 67 CASREACT COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 127:277975 CASREACT Full-text
 TITLE: Activated cyclooctenones are effective
 dienophiles
 AUTHOR(S): Liu, Hsing-Jang; Wang, Dan-Xiong; Kim, Jeung
 Beaj; Browne, Eric N. C.; Wang, Yu
 Dep. of Chem., Univ. of Alberta, Edmonton, AB,
 T6G 2G2, Can.
 SOURCE: Canadian Journal of Chemistry (1997
), 75(6), 899-912
 CODEN: CJCCHG; ISSN: 0008-4042
 PUBLISHER: National Research Council of Canada
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB The first Diels-Alder addition of a diene to a cyclooctenone dienophile has been observed. Three activated cyclooctenone dienophiles (I; R = H, R1 = Et; R = R1 = Me; R = Me, R1 = Et) are studied with a variety of simple and functionalized dienes. Diels-Alder adducts are produced in excellent yields under very mild Lewis acid catalyzed conditions. The usual orientation rules are followed, and, as predicted, the products are formed, for the most part, exclusively by ester-endo addition. The stereoselectivity is influenced by the substitution pattern of the diene in some cases. The factors influencing the stereochem. selectivity of the addition are discussed in some detail.

RX (39) OF 56 COMPOSED OF RX (24), RX (17)
 RX (39) AY + 2 AO + AQ + B ----> AE



RX (24) RCT AY 932-56-9, AO 616-38-6

STAGE (1)
 RCT AP 7646-69-7 NaH
 SOL 110-71-4 (CH2OMe)2

STAGE (2)
 RCT AO 64-19-7

STAGE (3)
 RCT AP 7646-69-7 NaH
 SOL 109-99-9 THF

STAGE (4)
 RCT AR 5707-04-0 PhSeCl
 SOL 109-99-9 THF

STAGE (5)
 RCT E 144-55-8 NaHCO3
 SOL 7732-18-5 Water, 60-29-7 Et2O

STAGE (6)
 RCT AL 7722-84-1 H2O2
 SOL 7732-18-5 Water

PRO Y 196398-71-7

RX (17) RCT Y 196398-71-7

STAGE (1)
 RCT D 7705-08-0 FeCl3

SOL 60-29-7 Et2O

STAGE(2)

RCT B 78-79-5

STAGE(3)

RGT E 144-55-8 NaHCO3
SOL 7732-18-5 WaterPRO AE 196398-86-4
REFERENCE COUNT: 24THERE ARE 24 CITED REFERENCES AVAILABLE
FOR THIS RECORD. ALL CITATIONS AVAILABLE
IN THE RE FORMATL74 ANSWER 12 OF 67 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1231142956 CASREACT Full-textTITLE: Selective transformations of alkynols
catalyzed by ruthenium complexes

AUTHOR(S):

Bruneau, Christian; Kapouche, Zahia; Neveux,
Muriel; Seillier, Benedicte; Dixneuf, Pierre H.
Laboratoire de Chimie de Coordination
Organique, URA CNRS 415, Université de Rennes,
Campus de Beaulieu, Rennes, 35042, Fr.
Inorganica Chimica Acta (1994),
222(1-2), 155-63
CODEN: ICHAA3; ISSN: 0020-1693

SOURCE:

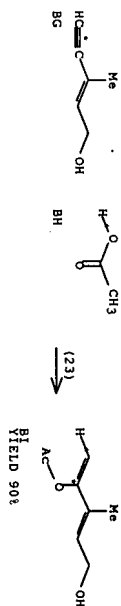
CODEN: ICHAA3; ISSN: 0020-1693
Journal

DOCUMENT TYPE:

LANGUAGE: English

AB Alkynols HC≡C(R)bond C≡CH2OH, HC≡C(R)bond C≡CH2CH2OH, and (E)-HC≡C(R)bond C≡CHCH2OH react with carboxylic acids in the presence of (Ru(μ-O2CH)(CO)2(PH)3)2 to selectively afford keto esters or trisubstituted hydroxy diethyl esters, depending on the possibility of effecting intramolecular transesterification. The potential of p-oxopropyl esters as mild acylating reagents and precursors of hydroxy amides, dipeptides, pseudodipeptides, polycarbonyl compounds, and acetylenic 1,2-diols has been shown.

RX(23) OF 30 BG + BH ==> BI



RX(23) RCT BG 6153-06-6, BH 64-19-7

STAGE(1)

CAT 151516-73-3 Ruthenium, tetracarbonylbis(μ-
(formato-KO:KO'))bis(triphenylphosphine)
(di-), (Ru-Ru)
SOL 108-88-3 PhMe

STAGE(2)

RGT D 144-55-8 NaHCO3

PRO BI 165945-58-0

L74 ANSWER 13 OF 67 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 116:214034 CASREACT Full-text

TITLE:

Enantioselective synthesis of cyclopentanoid
compounds from isoprene and diperylene
Baldenhus, Kai U.; Tom Dieck, Reinhold;
Koenig, Wilfried A.; Icheln, Detlef; Runge,
Torsten

CORPORATE SOURCE:

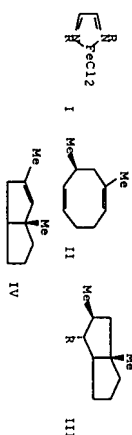
Inst. Angew. Chem., Univ. Hamburg,
Hamburg, W-2000/13, Germany
Angewandte Chemie (1992), 104(3),
338-40 (See also Angew. Chem., Int. Ed. Engl.,
1992, 31(3), 305-7)
CODEN: ANCEAD; ISSN: 0044-8249

SOURCE:

DOCUMENT TYPE:

LANGUAGE:

GI

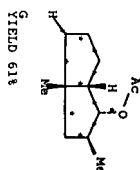


AB Cyclization of isoprene with piperylene in the presence of complex I (R = (1R)-menthyl) and butadienemagnesium-2-TiF gave 90% cyclooctadiene II, ee = 61%. Isomerization of II in the presence of an acid catalyst such as BF3·Et2O and an agent such as AcOH or PhH gave bicyclic compounds, such as III (R = OAc, Ph) and IV.

RX(5) OF 7 COMPOSED OF RX(1), RX(2)

RX(5) A + B + F ==> G





RX (1) RCT A 78-79-5, B 2004-70-8

PRO C 138541-38-5
CAT 87226-78-6 Iron, dichloro[N,N'-1,2-ethanediylidenebis(5-methyl-2-(1-methylethyl)cyclohexanamine)-N,N'-1-],

[7-4-[1R-[1a(1'R,2'S,5'R'),2b,5a]]]-,

83995-88-4 Magnesium, 2-butene-1,4-

diylbis(tetrahydrofuran)-, (T-4)-

NTE stereoselective

RX (2) RCT C 138541-38-5, F 64-19-7

PRO H 7664-93-9 H2SO4

PRO G 138541-39-6

SOL 64-19-7 AcOH

NTE stereoselective

L74 ANSWER 14 OF 67 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 116:20816 CASREACT Full-text
Title: Pigments of Fungi. XXI. Synthesis of

AUTHOR(S):

(z)-6-demethoxyaustrocortilubin
Burns, Christopher J.; Gill, Melvyn; Saubern,
Simon

CORPORATE SOURCE:

Sch. Chem., Univ. Melbourne, Parkville, 3052,
Australia

SOURCE:

Australian Journal of Chemistry (1991
, 44(10), 1427-45

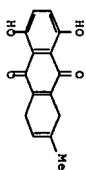
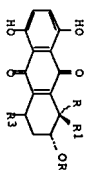
CODEN: AJCHAS; ISSN: 0004-9425

DOCUMENT TYPE:

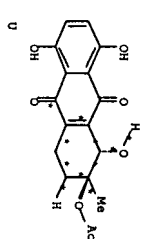
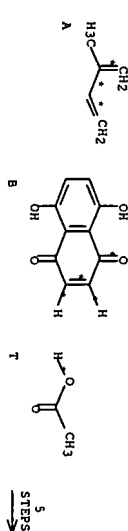
Journal

LANGUAGE: English

GI



AB 6-Demethoxyaustrocortilubin (I, R-R2 = H), is synthesized via the epoxide I (R2 = bond, R1, R3 = H) which is available in 73% yield over four steps from naphthazarin. Hydrolysis of I (R2 = bond, R1, R3 = H) yields the diol I (R, R2, R3 = H, R1 = OH) which on hydrogenolysis affords 6-demethoxy-1-deoxyaustrocortilubin (I, R-R3 = H). Stereoselective benzylidene hydroxylation of (I, R-R3 = H) gives I (R-R2 = H, R3 = OH). Cleavage of I (R2 = bond, R1, R3 = H) with AcOH-AcOH affords a mixture of the esters I (R = OAc, R1-R3 = H, R = OH, R1, R3 = H, R2 = Ac; R = R2 = R3 = H, R1 = OH), while methanolysis yields I (R = R2 = R3 = H, R1 = OMe) and its isomer. Hydrogenolysis of I (R = R2 = R3 = H, R1 = OAc, OMe; R = OH, R1 = R3 = H, R2 = Ac) gives high yields of I

RX (55) OF 62 COMPOSED OF RX (1), RX (3), RX (10), RX (11), RX (12)
RX (55) A + B + T ==> U

RX (1) RCT A 78-79-5, B 475-38-7

PRO C 14569-43-8

RX (3) RCT C 14569-43-8

RGT F 1310-73-2 NaOH

PRO E 65698-32-0

NTE H(+)

RX (10) RCT E 65698-32-0

RGT R 1493-13-6 F3CSO2H

PRO H 137788-35-3

RX (11) RCT M 137788-35-3

RGT H 937-14-4 MCPBA

PRO S 137788-36-4

RX (12) RCT S 137788-36-4, T 64-19-7

PRO U 137788-37-5

L74 ANSWER 15 OF 67 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 111:194066 CASREACT Full-text

Title: Acyloxyhalogenation of 1,3-diene hydrocarbons

AUTHOR(S):

Ivanov, S. V.; Stadenchuk, M. D.
Leningr. Tekhnol. Inst., Leningrad, USSR

CORPORATE SOURCE:

Zhurnal Obshchei Khimii (1989),
59(4), 865-73

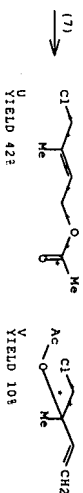
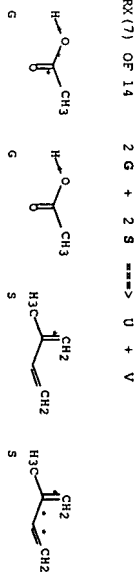
CODEN: ZORHA4; ISSN: 0044-460X

DOCUMENT TYPE:

Journal

LANGUAGE: Russian

AB Acyloxychlorination of divinyl with p-ClC6H4SO2NC12 in HCO2H, AcOH, MeCH2CO2H led to the resp. 1,2- and 1,4-addition products ClCH2CH:CHCH2O2CR and ClCH2CH(O2CR)CH:CH2 in comparable yields (i.e., 56:44 for R = H). LiClO4 was found to suppress the competing polymerization reaction, and enhances the 1,4-addition reaction. Acyloxyhalogenation of isoprene and CH2:CMcCM:CH2 was also studied. The authors warn of the possibility of explosion in the direct distillation of products from the reaction mixture, as well as the allergic nature of the reaction products.

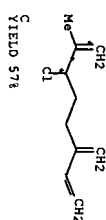
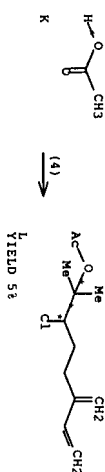
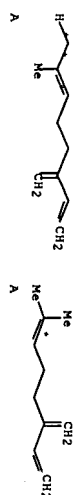


RX (7) RCT G 64-19-7, S 70-79-5
RGT E 17260-65-0 Benzenesulfonamide, N,N,4-trichloro-, F
7791-03-9 LiClO4
PRO U 38872-49-0, V 24517-68-8
SOL 64-19-7 AcOH

L74 ANSWER 16 OF 67 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 112:36192 CASREACT Full-text
TITLE: Formal ene-chlorination of myrcene by N-chlorosuccinimide
AUTHOR(S): Schulze, Klaus; Hauke, Guenter; Koehler, Gunther
CORPORATE SOURCE: Sekt. Chem., Karl-Marx-Univ., Leipzig, DDR-7010, Ger. Dem. Rep.
SOURCE: Zeitschrift fuer Chemie (1989), 29(5), 167-8
CODEN: ZECEAL; ISSN: 0044-2402

DOCUMENT TYPE: Journal
LANGUAGE: German
AB Reaction of myrcene with NCS in ROH (R = H, Me, Ac) containing H2SO4 gave Me2C(OR)CHClCH2CH2C(=CH2)CH:CH2 in 64, 38, and 5% yields, resp., along with 21-57% CH2:CMcCM:CH2CH2C(=CH2)CH:CH2 (1). I reacted with KSCN or NaOR (R = H, Ac, CHO) to give 44-80% CH2:CMcCM:CH2CH2CH2C(=CH2)CH:CH2 (R2 = SCN, R1).

RX (4) OF 29 2 A + K ==> L + C...

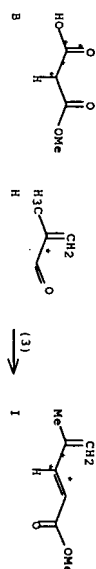


RX (4) RCT A 123-35-3, K 64-19-7
RGT D 128-09-6 Chlorosuccinimide
PRO L 124431-86-3, C 72420-53-2
CAT 7664-93-9 H2SO4
SOL 64-19-7 AcOH

L74 ANSWER 17 OF 67 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 110:74799 CASREACT Full-text
TITLE: An efficient one-pot preparation of 2,4-pentadienoic esters from α,β -unsaturated aldehydes
AUTHOR(S): Rodriguez, J.; Waegell, B.
CORPORATE SOURCE: Fac. Sci., St-Jerome, Univ. Aix-Marseille III, Marseille, F-13397, Fr., 534-5
SOURCE: Synthesis (1988), (7), 534-5
CODEN: SYNTHF; ISSN: 0039-7881

DOCUMENT TYPE: Journal
LANGUAGE: English
AB α,β -Unsaturated aldehydes reacted with monoalkyl malonate and pyridine with a catalytic amount of DMAP in a regio- and stereoselective process to yield almost exclusively 2,4-pentadienoic esters with essentially (and in many cases exclusively) the 2E-stereochem. Thus, HO2CCH2CO2Me and RCH:CR'CHO (R = H, Me, Ph, R1 = H; R = H, R1 = Me; R1 = CH:CHO) gave 84-100% RCH:CR'CH2CH2CH2CO2Me.

RX (3) OF 6 B + H ==> I

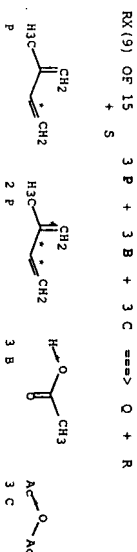


RX(3) RCT B 16695-14-0, H 78-85-3
RGT D 1122-58-3, 4-DMAP
PRO I 37974-16-6
SOL 110-86-1 Pyridine

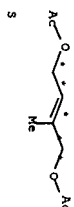
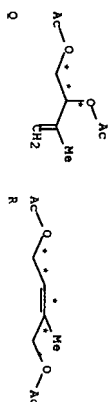
L74 ANSWER 18 OF 67 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 103:5870 CASREACT Full-text
TITLE: Liquid-phase 1,4-diacetoxylation of conjugated
dienes with tellurium(IV) oxide and alkali
metal halides

AUTHOR(S): Uemura, Sakeo, Fukuzawa, Shinichi; Patil,
Suresh R.; Okano, Masaya
CORPORATE SOURCE: Inst. Chem. Res., Kyoto Univ., Kyoto, 611,
Japan
SOURCE: Journal of the Chemical Society, Perkin
Transactions 1: Organic and Bio-Organic
Chemistry (1972-1999) (1985), (3),
499-503
CODEN: JCPR84; ISSN: 0300-922X

DOCUMENT TYPE: English
LANGUAGE: English
AB Oxidation of CH₂=C(R)CH=CH₂ (R = H, Me; R = H, Me) with TeO₂ in HOAc
containing LiBr gave isomeric mixts. of the corresponding diacetoxyalkene 1,2- and 1,4-
addition products; the product yields and selectivities were high in the presence of
excess LiBr. The reaction also occurred in the presence of NaBr, KBr, LiCl, HBr, or
Iodine, but yields and selectivities were lower. The mechanism is discussed.



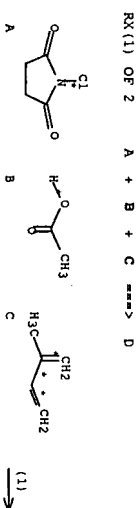
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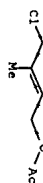
RX(9) RCT P 78-79-5, B 64-19-7, C 108-24-7
RGT G 7446-07-3 TeO₂, H 7550-35-8 LiBr
PRO Q 30264-53-0, R 59055-00-4, S 59054-99-8

L74 ANSWER 19 OF 67 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 98:142973 CASREACT Full-text
TITLE: 4-Chloro-3-methylcrotyl esters
Patent Assignee(s): Daihapon Ink and Chemicals, Inc., Japan;
Kawamura Physical and Chemical Research
Institute
SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 57183742	A	19821112		
PRIORITY APPLN. INFO.:				
JP 1981-65238		19810501		
AB RCOZCH ₂ CH:CHCH ₂ Cl (R = alkyl, aralkyl, Ph) were prepared by esterification of RCOZCH with isoprene and chlorinating agents. Thus, 18 g N-chlorosuccinimide was dissolved in 36 g HOAc at 45°, 13 g isoprene in HOAc added at 45-55°, and the solution heated at 50-55° to give 4.5 g trans-I (R = Me) and 3.0 g MeCOZCH ₂ CH:CHCH ₂ Cl.				



(11)



D

RX (1) RCT A 128-09-6, B 64-19-7, C 78-79-5
PRO D 38872-49-0

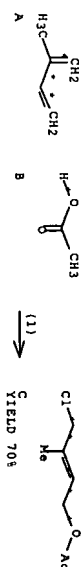
L74 ANSWER 20 OF 67 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 97:91789 CASREACT Full-text
TITLE: Stereospecific palladium-catalyzed
1,4-acetoxychlorination of 1,3-dienes
AUTHOR(S): Baekvall, Jan E.; Nordberg, Ruth E.;
Nyström, Jan E.
CORPORATE SOURCE: Dep. Org. Chem., R. Inst. Technol., Stockholm,
S-100 44, Sweden.
Tetrahedron Letters (1982), 23(15),
1617-20
CODEN: TETLEA; ISSN: 0040-4039

DOCUMENT TYPE: Journal
LANGUAGE: English
GI



AB Pd-catalyzed oxidation of cyclic and acyclic 1,3-dienes in AcOH in the presence of LiCl/LiOAc gave 1-acetoxy-4-chloro-2-alkenes with high selectivity. E.g., addition of cyclohexa-1,3-diene to a mixture of benzoinone, Pd(OAc)₂, and LiCl/LiOAc in AcOH over 3 h, followed by reaction at room temperature for 5 h, gave 89% of a >98:2 mixture of cyclohexenes I (R = β-, α-Cl, R1 = OAc). The mechanism involves π-allyl complex formation through (E)-acetoxy-palladation of 1 double bond followed by external (E)-attack by Cl-. The 1,4-adducts were stereo- and regioselectively functionalized. E.g., substitution reaction of I (R = β-Cl, R1 = OAc) with Me₂NH gave 93% I (R = α-Me₂N, R1 = OAc), which underwent substitution reaction with NaCH(CO₂Me)₂ to give 80% I (R = α-Me₂N, R1 = CH(CO₂Me)₂).

RX (1) OF 19 A + B ==> C...



RX (1) RCT A 78-79-5, B 64-19-7
PRO C 38872-49-0

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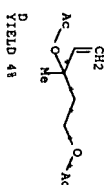
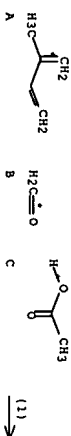
CAT 106-51-4 p-Benzoinone

L74 ANSWER 21 OF 67 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 98:71424 CASREACT Full-text
TITLE: Ruthenium-catalyzed Prins reaction
AUTHOR(S): Thivolle-Cazat, Jean; Tkatchenko, Igor
CORPORATE SOURCE: Inst. Rech. Catal., Villeurbanne, 69626, Fr.
Journal of the Chemical Society, Chemical
Communications (1982), (19), 1128-9
CODEN: JCCCAT; ISSN: 0022-4936

DOCUMENT TYPE: Journal
LANGUAGE: English

AB The preparation of 1,3-diol derivs. by the Prins reaction of dienes and alkenes with aldehydes and carboxylic acids was catalyzed by Ru salts. E.g., reaction of (H₂C=CH)₂ (I) with paraformaldehyde and MeCO₂H in the presence of RuCl₃ in the absence of solvent for 20 h gave a 5:23:10 mixture of 4-vinyl-m-dioxane (II) and H₂C=CHCH(OAc)(CH₂)₂OH (III); R = H, Ac) together with 17 parts oligomeric H₂C=CHCH(OAc)(CH₂)₂CH₂CH₂CH₂OH (IV). The ratio of cyclic product to oligomer varied with the reaction conditions. E.g., similar reaction in the presence MeONa for 20 h gave a 2.5:39.6:24 mixture of II, III (R = H, Ac), and IV.

RX (1) OF 1 A + B + C ==> D



RX (1) RCT A 78-79-5, B 50-00-0, C 64-19-7
PRO D 80118-03-2

L74 ANSWER 22 OF 67 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 97:145026 CASREACT Full-text
TITLE: Syntheses of dihydrolavandulol and its related compounds from carboxylic acids and conjugated dienes
AUTHOR(S): Fujita, Tsutomu; Watanabe, Shoji; Suga, Kyoichi; Maeda, Toshio; Suganaka, Kotoji; Kikuchi, Hajime
CORPORATE SOURCE: Dep. Appl. Chem., Chiba Univ., Chiba, 260, Japan

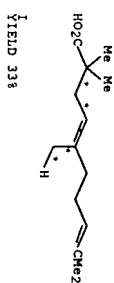
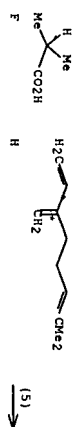
SOURCE: Journal of Chemical Technology and Biotechnology (1979-1982) (1982), 32(3), 476-84
CODEN: JCTBDC; ISSN: 0142-0356

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DOCUMENT TYPE: English
JOURNAL

AB Slow addition of isoprene in THF to 3-methylbutanoic acid, Me₂NCN:CHMe₂, and Na naphthalenide in THF under N at room temperature followed by refluxing 8 h and standing overnight gave 65% dihydroxylavandilic acid (I), LiAlH₄ reduction of which gave 85% title compound MeC:CHCH₂CH(CH₂OH)CHMe₂ (II). II is used in com. fragrances. Oxidation of II with pyridinium chlorochromate gave 81% dihydroxylavandulyl aldehyde (III). Cyclization of I with H₂SO₄ in C₆H₆ gave 82% 5,5-dimethyl-2-isopropyl-6-valerolactone (IV). Several analogs of I-IV were prepared similarly. 2-Alkyl- and 2,2-dialkyl-substituted 5-methyl-4-hexenols, 5-methyl-4-hexenals, and 5,5-dimethyl-5-pentanolides have sweet odors and can be used in perfumes.

RX (5) OF 103 F + H ==> I



RX (5) RCT F 79-31-2, H 123-35-3
PRO I 70777-58-1

L74 ANSWER 23 OF 67 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 96:199042 CASREACT Full-Text
TITLE: Selective 1,4-diacetoxylation of conjugated
diene with tellurium(IV) oxide

AUTHOR(S): Uemura, Sakae; Fukuzawa, Shinichi; Okano,
Masaya

CORPORATE SOURCE: Inst. Chem. Res., Kyoto Univ., Kyoto, 611,
Japan

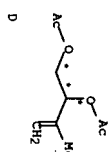
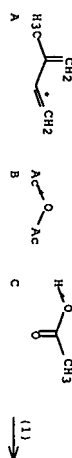
SOURCE: Tetrahedron Letters (1981), 22(52),
5331-4

DOCUMENT TYPE: English
JOURNAL

LANGUAGE: English

AB Oxidation of linear conjugated dienes with TiO₂ and LiBr in AcOH gave a mixture of 1,2- and 1,4-diacetoxyalkenes. When the ratio of LiBr to TiO₂ was 5-10 the 1,4-isomer was produced highly selectively. E.g., reaction of 5 equiv butadiene with AcOH-Ac₂O, 1 equiv TeO₂, and 5 equiv LiBr at 125° for 20 h gave a 1:9 mixture of CH₂:CHCH(OMe)CH₂OMe and (E)- and (Z)-AcOCH₂CH:CHCH₂OMe.

RX (1) OF 6 A + B + C ==> D



RX (1) RCT A 78-79-5, B 108-24-7, C 64-19-7
RCT E 7446-07-3 TeO₂, F 7550-35-8 LiBr
PRO D 30264-53-0

L74 ANSWER 24 OF 67 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 95:96978 CASREACT Full-Text
TITLE: Diacetoxylation of conjugated dienes with
tellurium(III) acetate in acetic acid

AUTHOR(S): Uemura, Sakae; Miyoshi, Haruo; Tabata, Akira;
Okano, Masaya

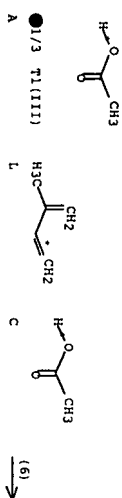
CORPORATE SOURCE: Inst. Chem. Res., Kyoto Univ., Kyoto, 611,
Japan

SOURCE: Tetrahedron (1981), 37(12), 291-5

DOCUMENT TYPE: English
JOURNAL

AB Conjugated dienes reacted with Ti(OMe)₃ in AcOH to give isomeric mixts. of the 1,2- and 1,4-diacetoxyalkene addition products. 1,2-Addition products predominated. E.g., CH₂:CHMe:CH₂ reacted with Ti(OMe)₃ (AcOH, 20°, 1 h) to give 71% of an 83:17 mixture of CH₂:CHMe:CH₂OMe and AcOCH₂CH:CHMe:CH₂OMe. The mechanism of the reaction is discussed.

RX (6) OF 11 A + L + C ==> M



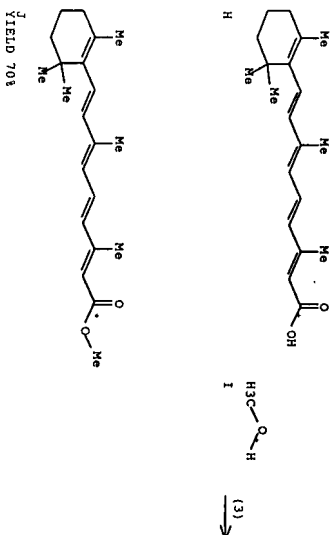
L74 ANSWER 25 OF 67 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 57:29994 CASREACT Full-text
TITLE: Synthesis of carboxylic acid esters by the

AUTHOR(S): Straab, Heinz A.; Mamschreck, Albrecht
CORPORATE SOURCE: Univ. Heidelberg, Germany
SOURCE: Chemische Berichte (1962), 95, 100-102

DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB The basecatalyzed imidazole method allowed the pr

The base-catalyzed imidazole method allowed the preparation of esters from carboxylic acids and alcohols at room temperature in extremely short reaction periods with very good yields. The new method was applied to the prepn. of esters from highly unsat. alcohols and carboxylic acids of the vitamin A series and the prepn. of esters of terpenes. Starting from N,N'-carbonylimidazole (I), sym. and unsym. esters of carboxylic acid were obtained, as well as imidazole-N-carboxylic acid esters, the pyrolysis of which yielded N-substituted imidazoles. Adipic acid dimidazolate (12.31 g.) (from equimolar amts. of adipic acid and I in tetrahydrofuran) treated at room temperature with stirring with 0.015 g. Na in 60 cc. in tetrahydrofuran, the mixture treated after 0.5 min. with 17 cc. 6.2N HCl, evaporated in vacuo, and the residue extracted with Et₂O yielded 7.35 g. BzC₁₀H₁₇CO₂ImE, b₁₂-5.13 112.5°, n_D20 1.4285. PhC₁₀H₁₇CO₂ImE (21.02 g.) in 70 cc. THF, refluxed with 0.20 g. Na, added at 20° to 33.73 g. N-benzoylimidazole (II) in 60 cc. Et₂O, and the extract worked up yielded 36.0 g. BzC₁₀H₁₇ (III), m. 1920°, d₁₅ 1.80-1.9. Na (0.20 g.) and 2.0 g. imidazole in 20 cc. THF, refluxed, cooled, treated with 21.02 g. PhC₁₀H₁₇ in 50 cc. THF, and processed in the usual manner yielded 34.1 g. III. I (27.88 g.) in 200 cc. THF, stirred 2 h. at room temperature with 20.0 g. BzOH and treated with a solution of 0.17 g. Na and 18.60 g. PhC₁₀H₁₇ in 80 cc. THF gave in the usual manner 30.7 g. III. N-Acetylimidazole (16.75 g.) in 150 cc. THF mixed with 15.70 g. PhC₁₀H₁₇CH₂OH, treated at room temperature with a soln. of 0.40 g. Na and 4.0 g. imidazole in 50 cc. THF, kept overnight, the residue shaken with the 3-fold amount of H₂O, and extracted with Et₂O yielded 20.25 g. PhC₁₀H₁₇CH₂CO₂ImE, b₁₅ 139-41.5°, n_D20 1.5428. PhC₁₀H₁₇CH₂CO₂ImE in 30 cc. THF, added at room temperature to 0.40 g. Na and 4.0 g. imidazole in 40 cc. THF, the mixture treated with 21.25 g. II in 50 cc. THF, kept overnight, and worked up gave 22.75 g. PhC₁₀H₁₇CH₂CO₂ImE, m. 39-9.5°, b₁₀ 137-8.5°. I (19.89 g.) in 100 cc. THF, stirred 2 h. with 14.30 g. BzOH and added at room temperature to 0.40 g. Na, 4.0 g. imidazole, and 15.71 g. PhC₁₀H₁₇CH₂OH in 80 cc. THF, and worked up yielded 21.81 g. PhC₁₀H₁₇CH₂CO₂ImE. PhC₁₀H₁₇CH₂CO₂ImE (2.80 g.) in 25 cc. THF, added at room temperature to 0.10 g. Na and 2.0 g. imidazole dissolved in 15 cc. THF, the mixture treated with 7.10 g. N-pivaloylimidazole in 100 cc. THF, kept at room temperature overnight and some time at 50°, evaporated, the residue ground with 250 cc. N NaOH, kept 6 h., filtered, and the filtrate worked up yielded 6.19 g. C₁₅H₂₁CO₂CHC₁₀H₁₇CH₂OH, leaflets, m. 46-6.5° (EtOH). PhC₁₀H₁₇CH₂CO₂ImE (14.08 g.) in 150 cc. THF, stirred 1 h. with 16.20 g. I, treated with 0.46 g. Na in 5.0 g. MeOH, evaporated after 1 h., the residue shaken with 200 cc. H₂O, and the aqueous solution extracted with Et₂O yielded 11.05 g. PhC₁₀H₁₇CH₂CO₂ImE, m. 34-5.5°, d₁₅ 132.5-34°. and 1.0 g. imidazole in 100 cc. THF under N treated successively with 2.20 g. N-acetylimidazole in 80 cc. THF and 2.91 g. Vitamin A (IV) in 27 cc. THF, stirred 2 h., evaporated, the residue kept with H₂O overnight, extracted with Et₂O, and the extract worked up yielded 2.17 g.

RX(3) OF 5 H + I -> J



RX(3) RCT H 302-79-4, I 67-56-1
RGT F 530-62-1 Dimidazolyl ketone
PRO J 333-16-2

SOL 71-43-2 Benzene, 67-56-1 MeOH
NTE Classification: Esterification; Alkoxylation; #
Conditions: carbodimidazole, benzene 4h; several mm Rf;
NaOMe MeOH; overnight/NZ

REENTER DISPLAY FORMAT FOR ALL FILES (FILEDEFAULT):

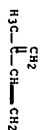
=> d 174 26-67 ibid ed abs hltstr hltind

I74 ANSWER 26 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:76041 HCAPLUS Full-text
DOCUMENT NUMBER: 140:63804
TITLE: Protocol for the development of the master
chemical mechanism, MCM v3 (part A):
tropospheric degradation of non-aromatic
volatile organic compounds
Saunders, S. M.; Jenkin, M. E.; Derwent, R.
G.; Pilling, M. J.
School of Chemistry, University of Leeds,
Leeds, LS2 9JT, UK
Atmospheric Chemistry and Physics (2003), 3(1), 161-180
CODEN: ACPTCE; ISSN: 1680-7324
PUBLISHER: European Geophysical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

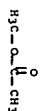
ED Entered STN: 29 Sep 2003
AB Kinetic and mechanistic data relevant to the tropospheric degradation of volatile organic compounds (VOC), and the production of secondary pollutants, were previously used to define a protocol which underpinned the construction of a near-explicit Master Chemical Mechanism. An update to the previous protocol is presented, which was used to

define degradation schemes for 107 nonarom. VOC as part of version 3 of the Master Chemical Mechanism (MCM v3). The treatment of 18 aromatic VOC is described in a companion paper. The protocol is divided into subsections describing initiation reactions, the reactions of the radical intermediates and the further degradation of 1st and subsequent generation products. Emphasis is placed on updating the previous information, and outlining the methodol. which is specifically applicable to VOC not considered previously (e.g., α - and β -pinene). The present protocol aims to take into consideration work available in the open literature up to the beginning of 2001, and some other studies known by the authors which were under review at the time. Application of MCM v3 in appropriate box models indicates that the representation of isoprene degradation provides a good description of the speciated distribution of oxygenated organic products observed in reported field studies where isoprene was the dominant emitted hydrocarbon, and that the α -pinene degradation chemical provides a good description of the time dependence of key gas phase species in α -pinene/NOx photooxidn. expts. carried out in the European Photoactor (EUPHORE). Photochem. Ozone Creation Potentials (POCP) were calculated for the 106 non-aromatic non-methane VOC in MCM v3 for idealized conditions appropriate to north-west Europe, using a photochem. trajectory model. The POCP values provide a measure of the relative ozone forming abilities of the VOC. Where applicable, the values are compared with those calculated with previous versions of the MCM.

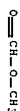
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, Methyl acetate 107-31-3, Methyl formate 109-60-4, n-Propyl acetate 123-86-4, n-Butyl acetate 141-78-6, Ethyl acetate, reactions 540-88-5, tert-Butyl acetate
Rf: POL (Pollutant); RCT (Reactant); OCCU (Occurrence); RACT (Reactant or reagent)
(tropospheric degradation of non-aromatic volatile organic compds.)
RN 78-79-5 HCAPLUS
CN 1,3-Butadiene, 2-methyl- (CA INDEX NAME)



RN 79-20-9 HCAPLUS
CN Acetic acid, methyl ester (CA INDEX NAME)



RN 107-31-3 HCAPLUS
CN Formic acid, methyl ester (CA INDEX NAME)



RN 109-60-4 HCAPLUS
CN Acetic acid, propyl ester (CA INDEX NAME)



CN 123-86-4 HCAPUS
 Acetic acid, butyl ester (CA INDEX NAME)

 n-Bu-O-Ac

 Et-O-Ac

 RN 141-78-6 HCAPUS
 Acetic acid ethyl ester (CA INDEX NAME)

 Et-O-Ac

 RN 540-88-5 HCAPUS
 Acetic acid, 1,1-dimethylethyl ester (CA INDEX NAME)

 t-Bu-O-Ac

 CC 59-2 (Air Pollution and Industrial Hygiene)
 Section cross-reference(s): 53
 50-00-0, Methanol, reactions 57-55-6, 1,2-Propanediol, reactions
 60-29-7, Diethyl ether, reactions 64-17-5, Ethanol, reactions
 64-18-1, Formic acid, reactions 64-19-7, Acetic acid, reactions
 67-56-1, Methanol, reactions 67-63-0, Propan-2-ol, reactions
 67-64-1, Propanone, reactions 67-66-3, Trichloroethane,
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 reactions 74-87-3, Chloromethane, reactions 74-98-6, Propane,
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 2-Methylpropan-2-ol, reactions 75-83-2, 2,2-Dimethylbutane
 75-85-4, 2-Methylbutan-2-ol 75-97-8, 3,3-Dimethylbutan-2-one
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 reactions 79-09-4, Propanoic acid, reactions 79-20-9,
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 α-Pinene 96-14-0, 3-Methylpentane 96-22-0, Pentan-3-one
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 106-98-9, But-1-ene, reactions 106-99-0, Buta-1,3-diene,
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 1-Methoxypropan-2-ol 108-10-1, 4-Methylpentan-2-one 108-20-3,
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 Cyclohexanone, reactions 109-60-4, n-Propyl acetate
 109-66-0, Pentane, reactions 109-67-1, Pent-1-ene 109-86-4,
 2-Methoxyethanol 109-87-5, Dimethoxymethane 110-54-3, Hexane,
 reactions 110-62-3, Pentanal 110-80-5, 2-Ethoxyethanol,
 reactions 110-82-7, Cyclohexane, reactions 111-65-9, Octane, reactions
 111-76-2, 2-Butoxyethanol 111-84-2, Nonane 112-40-3, Dodecane
 115-07-1, Propene, reactions 115-10-6, Dimethyl ether
 115-11-7, 2-Methylpropane, reactions 123-38-6, Propanal,
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3-Methylbutan-1-ol 123-72-8, Butanal 123-66-4, n-Butyl
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 141-46-8 141-78-6, Ethyl acetate, reactions 142-82-3,
 Heptane, reactions 156-59-2, cis-1,2-Dichloroethene 156-60-5,
 trans-1,2-Dichloroethene 163-82-1, 2,2-Dimethylpropane
 513-35-9, 2-Methylbut-2-ene 540-88-5, tert-Butyl acetate
 563-45-1, 3-Methylbut-1-ene 563-46-2, 2-Methylbut-1-ene
 563-79-1, 2,3-Dimethylbut-2-ene 563-80-4, 3-Methylbutan-2-one
 584-02-1, Pentan-3-ol 589-34-4, 3-Methylhexane 589-38-8,
 Hexan-3-one 590-18-1, cis-But-2-ene 591-76-4, 2-Methylhexane
 591-78-6, Hexan-2-one 592-41-6, Hex-1-ene, reactions 598-75-4,
 3-Methylbutan-2-ol 616-38-6, Carbonic acid, dimethyl ester
 624-64-6, trans-But-2-ene 627-20-3, cis-Pent-2-ene 637-92-3
 646-04-8, trans-Pent-2-ene 1120-21-4, Undecane 1634-04-4,
 Methyl tert-butyl ether 2278-22-0, Peroxyacetyl nitrate
 4050-45-7, trans-Hex-2-ene 5131-66-8, 1-Butoxypropan-2-ol
 7688-21-3, cis-Hex-2-ene 10102-43-9, Nitrogen oxide no,
 reactions 10102-44-0, Nitrogen oxide no2, reactions
 11104-93-1, Nox, reactions 88181-75-3
 RL: POL (Pollutant); RCT (Reactant); OCCU (Occurrence); RACT
 (Reactant or reagent)
 (tropospheric degradation of non-aromatic volatile organic compds.)
 REFERENCE COUNT: 98
 THERE ARE 98 CITED REFERENCES AVAILABLE
 FOR THIS RECORD. ALL CITATIONS AVAILABLE
 IN THE RE FORMAT

L74 ANSWER 27 OF 67 HCAPUS COPYRIGHT 2007 ACS ON STN
 ACCESSION NUMBER: 2003:34333 HCAPUS Full-text
 DOCUMENT NUMBER: 139:89246
 TITLE:
 Speciation of volatile organic compound
 emissions for regional air quality modeling of
 particulate matter and ozone
 AUTHOR(S):
 Makar, P. A.; Moran, M. D.; Scholtz, M. T.;
 Taylor, A.
 CORPORATE SOURCE:
 Modelling and Integration Division, Air
 Quality Research Branch, Meteorological
 Service of Canada, Toronto, ON, Can.
 SOURCE:
 Journal of Geophysical Research, [Atmospheres]
 (2003), 108(D2), ACH 2/1-ACH 2/51
 CODEN: JGRD33; ISSN: 0148-0227
 PUBLISHER:
 American Geophysical Union
 LANGUAGE:
 English
 ED Entered STN: 08 May 2003
 AB A new classification scheme for speciation of organic compound emissions for use in air
 quality models is described. This scheme uses 81 organic compound classes to preserve
 net gas-phase reactivity and particulate matter (PM) formation potential. Chemical
 structure, vapor pressure, OH- reactivity, i.p./b.p., and solubility data were used to
 create the 81 compound classes. Volatile, semi-volatile, and non-volatile organic
 compounds are included. This classification scheme was used in conjunction with the
 Canadian Emissions Processing System (CEPS) to process 1990 gas- and particle-phase
 organic compound emissions data for summer and winter for a domain covering much of
 eastern North America. A simple post-processing model analyzed speciated organic
 emissions in terms of gas-phase reactivity and potential to form organic PM.
 Previously unresolved compound classes which may significantly affect O3 formation
 included biogenic high-reactivity esters and internal C5-8 alkenes-alcs, and
 anthropogenic ethanol and propanol. Organic radical production associated with
 anthropogenic organic compound emissions may be 21 orders of magnitude more important
 than biogenic-associated production in northern US and Canadian cities, and a factor
 of 3 more important in southern US cities. Previously unresolved organic compound
 classes, e.g., low vapor pressure polycyclic aromatic hydrocarbons (PAH), anthropogenic
 diacids, dialkyl phthalates, and high C number alkanes, may have a significant impact
 on organic particle formation. Primary organic particles (poorly characterized in
 national emissions databases) dominate total organic particle concns., followed by
 secondary formation and primary gas-particle partitioning. The effect of the assumed

Initial aerosol water concentration on subsequent thermodyn. calcs. suggested hydrophobic and hydrophilic compds. may form external mixts., and that sep. treatment for these groups may be required in future air quality model simulations. The post-processing model used overestimated organic particle formation relative to measurements, lacked the complexity of a regional air quality model, and was not intended as an alternative to the latter. However, post-processing model results do provide guidance for treating organic gases and particles in future air quality modeling work. Future air quality model simulations should attempt to speciate primary particulate organic compds. and include more detailed organic compound classes. Future emissions profile measurements should speculate gaseous high mol. mass organic compds. and primary orgs. emitted in particulate form (primary particle emissions are only available as a total particulate mass in currently available missions data).

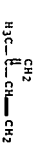
IT

78-79-5, Isoprene, reactions 79-20-9, Methyldiacrylate 84-74-2, Dibutylphthalate 85-68-7, Butylbenzylphthalate 96-33-3, Methyldiacrylate 105-37-3 106-65-0, Dimethylbutanedioate 107-31-3, Methylformate 108-05-4 Vinyl acetate, reactions 108-21-4 Isopropyl acetate 109-60-4, n-Propylacetate 110-19-0, Isobutylacetate 111-19-9, Cellosolve acetate 111-82-0, Methyl dodecanoate 112-39-0, Methylpalmitate 112-61-8, Methyl stearate 120-61-6, Dimethylterephthalate 123-35-3, Myrcene 123-66-0, Ethylhexanoate 123-86-4, n-Butylacetate 124-10-7, Methyl myristate 131-11-3, Dimethylphthalate 136-60-7, Butylbenzoate 140-88-5, Ethylacrylate 141-32-2, Butylacrylate 141-78-6, Ethylacetate, reactions 547-63-7, Methyl isobutylate 627-93-0, Dimethylhexanedioate 119-40-0, Dimethyl pentanedioate RI: OCCU (Occurrence); BACT (Reactant or reagent) (Reactant); OCCU (Occurrence); POL (Pollutant); RCT (volatile organic compound emission speciation for modeling regional air quality and particulate matter and ozone formation)

RN

78-79-5 HCAPLUS

CN 1,3-Butadiene, 2-methyl- (CA INDEX NAME)



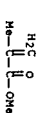
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CN Acetic acid, methyl ester (CA INDEX NAME)



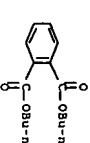
RN 80-62-6 HCAPLUS

CN 2-Propenoic acid, 2-methyl-, methyl ester (CA INDEX NAME)



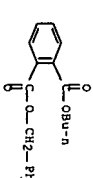
RN 84-74-2 HCAPLUS

CN 1,2-Benzenedicarboxylic acid, 1,2-dibutyl ester (CA INDEX NAME)



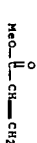
RN 85-68-7 HCAPLUS

CN 1,2-Benzenedicarboxylic acid, 1-butyl 2-(phenylmethyl) ester (CA INDEX NAME)



RN 96-33-3 HCAPLUS

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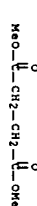
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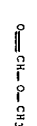
RN 106-65-0 HCAPLUS

CN Butenedioic acid, 1,4-dimethyl ester (CA INDEX NAME)

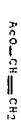


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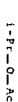
CN Formic acid, methyl ester (CA INDEX NAME)



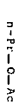
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CN Acetic acid ethenyl ester (CA INDEX NAME)



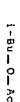
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CN Acetic acid, 1-methylethyl ester (CA INDEX NAME)



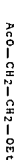
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CN Acetic acid, propyl ester (CA INDEX NAME)



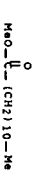
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CN Acetic acid, 2-methylpropyl ester (CA INDEX NAME)



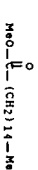
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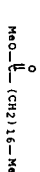
RN 111-82-0 HCAPLUS
CN Dodecanoic acid, methyl ester (CA INDEX NAME)



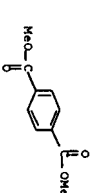
RN 112-39-0 HCAPLUS
CN Hexadecanoic acid, methyl ester (CA INDEX NAME)



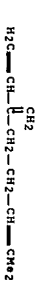
RN 112-61-8 HCAPLUS
CN Octadecanoic acid, methyl ester (CA INDEX NAME)



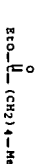
RN 120-61-6 HCAPLUS
CN 1,4-Benzenedicarboxylic acid, 1,4-dimethyl ester (CA INDEX NAME)



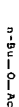
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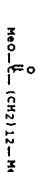
RN 123-66-0 HCAPLUS
CN Hexanoic acid, ethyl ester (CA INDEX NAME)



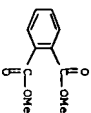
RN 123-86-4 HCAPLUS
CN Acetic acid, butyl ester (CA INDEX NAME)



RN 124-10-7 HCAPLUS
CN Tetradecanoic acid, methyl ester (CA INDEX NAME)



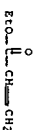
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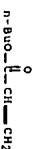
RN 136-60-7 HCAPLUS
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RN 140-88-5 HCAPLUS
 CN 2-Propenoic acid, ethyl ester (CA INDEX NAME)



RN 141-32-2 HCAPLUS
 CN 2-Propenoic acid, butyl ester (CA INDEX NAME)



RN 141-78-6 HCAPLUS
 CN Acetic acid ethyl ester (CA INDEX NAME)



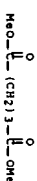
RN 547-63-7 HCAPLUS
 CN Propanoic acid, 2-methyl-, methyl ester (CA INDEX NAME)



RN 627-93-0 HCAPLUS
 CN Hexanedioic acid, 1,6-dimethyl ester (CA INDEX NAME)



RN 1119-40-0 HCAPLUS
 CN Pentanedioic acid, 1,5-dimethyl ester (CA INDEX NAME)



CC 59-2 (Air Pollution and Industrial Hygiene)

Section cross-reference(s): 53
 IT Aldehydes, reactions

Alkanes, reactions
 Alkenes, reactions
 Alkynes, reactions
 Amides, reactions
 Amines, reactions
 Carbonyl compounds (organic), reactions
 Epoxides
 Esters, reactions
 Ethers, reactions
 Hydrocarbons, reactions
 Ketones, reactions
 Naphtha
 Naphthenic acids, reactions
 Petroleum spirites
 Polyoxalkylenes, reactions
 Polysiloxanes, reactions
 Terpenes, reactions
 Thiols, reactions
 Volatile organic compounds

RL: OCU (Occurrence, unclassified); POL (Pollutant); RCT
 (Reactant); OCCU (Occurrence); RACT (Reactant or reagent)
 (volatile organic compound emission speciation for modeling regional
 air quality and particulate matter and ozone formation)

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RL: OCU (Occurrence, unclassified); POL (Pollutant); RCT (Reactant); OCCU (Occurrence); RCT (Reactant or reagent) (volatiles organic compound emission speciation for modeling regional air quality and particulate matter and ozone formation)

IT

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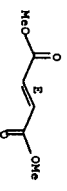
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Dichlorobenzene
Rt: OCU (Occurrence, unclassified); POL (Pollutant); RCT
(Reactant); OCCU (Occurrence); RACT (Reactant or reagent)

(volatile organic compound emission speciation for modeling regional
air quality and particulate matter and ozone formation)
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FOR THIS RECORD. ALL CITATIONS AVAILABLE
IN THE RE FORMAT

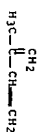
L74 ANSWER 28 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:181452 HCAPLUS FULL-TEXT
DOCUMENT NUMBER: 140:181474
TITLE: Product subclass 2: palladium-allyl complexes.
AUTHOR(S): Friesen, R. W.
CORPORATE SOURCE: Merck Frost Centre for Therapeutic Research,
Kirkland, PE, H9H 3J1, Can.
SOURCE: Science of Synthesis (2002), 1,
113-284
CODEN: SSCYJ9
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
ED Entered STN: 21 Nov 2002
AB A review on preparation and application of palladium-allyl complexes.
IT 116-17-6, Triisopropyl phosphite 624-49-7,
Dimethyl fumarate
Rt: CAT (Catalyst and application); USES (Uses)
(preparation and application of palladium-allyl complexes)
CN 116-17-6 HCAPLUS
CN Phosphorous acid, tris(1-methylethyl) ester (CA INDEX NAME)

OPr-1
1-PRO-1-OPr-1

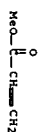
RN 624-49-7 HCAPLUS
CN 2-Butenedioic acid (2E)-, 1,4-dimethyl ester (CA INDEX NAME)
Double bond geometry as shown.



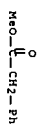
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141-12-8, Neryl acetate 141-97-9, Ethyl
acetoacetate 591-87-7, Allyl acetate 996-82-7,
Diethyl sodiomalonate 1191-16-8, 3-Methyl-2-butenyl
acetate 10544-63-5, Ethyl 2-butenolate 18424-76-5
, Dimethyl sodiomalonate
Rt: RCT (Reactant); RACT (Reactant or reagent)
Rt: (preparation and application of palladium-allyl complexes)
CN 78-79-5 HCAPLUS
CN 1,3-Butadiene, 2-methyl- (CA INDEX NAME)



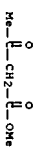
RN 96-33-3 HCAPLUS
CN 2-Propenoic acid, methyl ester (CA INDEX NAME)



RN 101-41-7 HCAPLUS
CN Benzenoacetic acid, methyl ester (CA INDEX NAME)

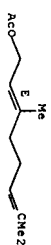


RN 105-45-3 HCAPLUS
CN Butanoic acid, 3-oxo-, methyl ester (CA INDEX NAME)



RN 105-87-3 HCAPLUS
CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2E) - (CA INDEX NAME)

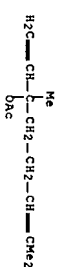
Double bond geometry as shown.



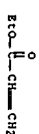
RN 108-59-8 HCAPLUS
CN Propanedioic acid, 1,3-dimethyl ester (CA INDEX NAME)



RN 115-95-7 HCAPLUS
CN 1,6-Octadien-3-ol, 3,7-dimethyl-, 3-acetate (CA INDEX NAME)



RN 140-88-5 HCAPLUS
CN 2-Propenoic acid, ethyl ester (CA INDEX NAME)

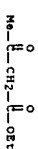


RN 141-12-8 HCAPLUS
CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2Z) - (CA INDEX NAME)

Double bond geometry as shown.



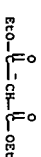
RN 141-97-9 HCAPLUS
CN Butanoic acid, 3-oxo-, ethyl ester (CA INDEX NAME)



RN 591-87-7 HCAPLUS
CN Acetic acid, 2-propen-1-yl ester (CA INDEX NAME)



RN 996-82-7 HCAPLUS
CN Propanedioic acid, 1,3-diethyl ester, ion(1-), sodium (1:1) (CA INDEX NAME)



RN 1191-16-8 HCAPLUS
CN 2-Buten-1-ol, 3-methyl-, 1-acetate (CA INDEX NAME)

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Cholesteryl- γ -3-one 603-35-0, Triphenylphosphine, reactions
603-35-0D, Triphenylphosphine, reaction product from palladium
dichloride dppc complex and DIBAL-H, 603-92-9, Dimethyl
methylmalonate 614-20-0 614-47-1, (E)-Benzylidenacetophenone
515-99-6, Diallyl oxalate 618-41-7, Phenylsulfonic acid
623-43-8 627-20-3, 2,1,2-Pentene 628-08-0, 2-Butenylic acetate
629-20-9, Cyclooctatetraene 614-82-8, Diketene 689-06-5
4-Methyl-3-hexen-2-one 693-86-7, Vinylcyclopropane 693-89-0,
1-Methylcyclopentene 754-05-2, Trimethylvinylsilane 754-06-3,
Trimethyl(vinyl)stannane 762-72-1, Allyltrimethylsilane
762-72-2, Allyldimethylstannane 763-29-1, 2-Methyl-1-pentene
765-69-3, 2-Methyl-1,1-methylcyclohexadiene 820-07-5, Methylallyl
formate 820-07-1, Methylallyl acetate 824-99-3, Sodium

p-toluenesulfonate 826-13-1, 827-69-0, 4-Phenylpent-3-en-2-one
827-87-2, 869-29-4, 873-55-2, Sodium phenylsulfinate
917-54-4D, Methylaluminum, reaction products with nickel
tetraacarbonyl 926-56-7, 4-Methyl-1,3-pentadiene 930-22-3,
Vinylcyclohexene 930-30-3, 2-Cyclopenten-1-one 934-56-5, 993-07-7,
Trimethylphenyltin 960-16-7, Tributylphenylstannane
1000-66-8, 2,4-Dimethyl-1,3-pentadiene 1072-25-9, Heptylallene
1074-24-4, Potassium phthalimide 1167-33-5, 1184-88-9, Sodium
pivalate 1189-09-9, Methyl (E)-geranate 1191-16-8,
3-Methyl-2-butenyl acetate 1192-37-6, Methylenechlorohexane
1196-73-2, 1205-42-1, 1424-22-2, 1450-14-2, Hexamethyldisilane
1458-99-7, 4-Chloropent-2-ene 1461-22-9, Tributylchlorostannane
1469-70-1, Allyl ethyl carbonate 1489-57-2, 2-Methyl-1,3-
cyclohexadiene 1521-51-3, 3-Bromocyclohexene 1528-30-9,
Methylenechloropentane 1541-29-3, 1576-98-3, 1617-18-1, Ethyl
3-butenolate 1617-19-2, Ethyl 3-methyl-3-butenolate 1700-10-3,
1,3-Cyclooctadiene 1746-13-0, Allyl phenyl ether 1809-67-2,
1896-62-4, 2001-45-8, Tetraphenylphosphonium chloride
2004-70-8, (E)-1,3-Pentadiene 2327-97-1, 1-Phenyl-1,2-pentadiene
2327-99-3, Phenylallene 2384-90-9, Butylallene 2442-10-6
2483-57-0, Methyl nitroacetate 2497-18-9, 2622-05-1,
Allylmagnesium chloride 2622-21-1, 1-Vinyl-1-cyclohexene
2637-34-5, 2-Sulfanylpiperidine 2664-62-0, Diazoacetone
2687-12-9, 3-Phenylallyl chloride 2749-96-4, p-Tolylallene
2783-10-0, 5-Methylhexa-1,3-diene 2923-17-3, Lithium
trifluoroacetate 2966-50-9, Silver(I) trifluoroacetate
3066-75-9, Allyl diethyl phosphate 3282-32-4, Phenyl diazomethyl
ketone 3618-12-0, Cyclohexene 3796-70-1, Geranylacetone
4054-38-0, 1,3-Cyclohexadiene 4074-22-0, 1,4-Dimethyl-1,4-
cyclohexadiene 4083-64-1, Tosyl isocyanate 4112-09-8
4157-02-2, 4356-59-2, 4372-94-5, 1,1-Dimethyl-2-ethoxyethane
4485-16-9, 4-Methyl-3-heptene 4497-92-1, (1)-2-Carene
4663-62-3, 4720-83-6, 6-Oxabicyclo[3.2.1]oct-3-en-7-one
4736-61-2, (2)-3-Methoxy-19-norpregna-1,3,5(10),17(20)-tetraene
4883-67-4, 2-Nitrocyclohexanone 4894-61-5, (E)-1-Chlorobut-2-ene
4964-03-8, (E)-1-(Trimethylsilyl)prop-1-ene 5194-50-3,
(E,2)-Hexa-2,4-diene 5194-51-4, (E,E)-Hexa-2,4-diene
5389-87-7, Geranyl chloride 5395-20-0, Benzyl p-Tolyl sulfone
5459-93-0, 5489-14-5, Silver(I) propionate 5674-01-1,
2-Methylallylmagnesium chloride 5732-13-8, 6088-88-6,
2-Butenylmagnesium chloride 6108-61-8, (Z,2)-Hexa-2,4-diene
6117-81-5, 2-Buten-1-ol 6142-73-0, Methylenechloropentane
6279-86-3, 6290-05-7, N,N-Bis(ethoxycarbonylmethyl)amine
6278-84-2, 6651-36-1, 6690-12-6, 9-Oxabicyclo[6.1.0]non-2-ene
6705-51-7, 7-Oxabicyclo[4.1.0]hept-2-ene 6737-11-7, 6790-37-0,
3,4-Epoxy-1-pentene 6790-38-1, Allyloxirane 6921-34-2,
Benzylmagnesium chloride 7129-41-1, 6-Oxabicyclo[3.1.0]hex-2-ene
7202-29-7, 7217-71-2, 7299-28-7, Tributyltin trifluoroacetate
7422-28-8, 7437-61-8, 7770-41-4, 10544-63-5, Ethyl
2-butenolate 12077-82-6, Bis[(η³-allyl)(μ-bromo)palladium]
12081-43-5, Bis[μ-bromo(η³-2-butenyl)palladium]
12103-44-1, 12138-25-5, 12211-09-1, 12463-39-3D, Nickel
tetracarbonyl, reaction products and methylaluminum or
benzylmagnesium chloride 13466-78-9, 3-Carene 13505-10-7,
5-Methyl-4-hexen-3-one 14155-77-2, Allylmercury chloride
14219-80-0, Thallium acetate 14309-16-1, 14371-10-9,
14483-67-1, tert-Butyl (trimethylsilyl) sulfide 14592-55-4,
Bis(acetonitrile)dichloropalladium 14750-79-9, 15022-08-9,
Diallyl carbamate 15525-45-8, Diallylurea tetrachloropalladate
16510-49-9, 1,2,3-Triphenylcyclopropane 16732-86-8,
M-Cholestene 16733-87-4, Cyclopentadienylaluminum
17094-21-2, 17351-28-9, 1,2-Dimethyl-1,4-cyclohexadiene
17442-12-7, 17447-60-8, 17851-97-7, 18025-87-4,
1,1,1-Trichloro-2,2,2-trimethylsilane 18424-76-5,

Diethyl sodiomalonate 18522-92-4, 18709-01-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(Preparation and application of palladium-allyl complexes)
100-52-7P, Benzaldehyde, preparation 123-35-3P,
β-Myrcene 930-68-7P, 2-Cyclohexen-1-one 1121-18-2P,
2-Methyl-2-cyclohexen-1-one 3112-87-6P, Allyl p-Tolyl sulfone
3724-55-8P, Methyl 3-butenolate 12081-18-4P, Bis[μ-
chloro(η³-2-methylallyl)palladium] 12081-22-0P,
Bis[(η³-2-butenyl)(μ-chloro)palladium] 14447-34-8P
16339-57-4P, (E)-1-Phenyl-1,3-butadiene 20657-21-0P
33306-44-5P, 2-Butenyl p-Tolyl sulfone 32007-86-6P
33306-44-5P, 33598-93-7P, Tributyltin chloride 33067-94-8P
53789-96-1P, 53789-97-2P, 53820-06-9P, 55883-94-8P
76166-46-6P, 77773-11-6P, 77944-71-9P, 87567-12-2P
88076-44-2P, 91443-64-0P, 95177-49-4P, 95177-50-7P
100898-93-9P, 656837-12-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP
(Preparation); RACT (Reactant or reagent)
(Preparation and application of palladium-allyl complexes)
94-66-6P, 104-55-2P, Cinamaldehyde 111-13-7P, Hexyl methyl
ketone 122-57-6P, 502-61-4P, (3E,6E)-α-Farnesene
601-11-6P, 5α-Cholest-2-en-1-one 601-55-8P,
5α-Cholest-1-en-3-one 818-58-6P, 877-94-1P,
5-Phenylpent-4-en-2-one 934-10-1P, 935-00-2P, 936-58-3P
936-67-4P, 2-Methylcyclohexanone 1002-35-3P, 1,3,7-Octatriene
1117-65-3P, 1120-73-6P, 2-Methylcyclopent-2-en-1-one 1123-34-8P
1205-84-1P, (E)-Ethyl 4-phenyl-3-butenolate 1208-44-2P
1271-03-0P, (η³-Allyl)(η⁵-cyclopentadienyl)palladium
1489-50-5P, 2-Methylenechloropent-1-one 1576-88-7P
1674-08-4P, trans-Biocarveol 1754-62-7P, 2436-90-0P
2482-22-0P, 2609-23-9P, 3045-76-9P, 3045-98-5P, 3338-55-1P
3393-45-1P, 3491-26-7P, 3491-27-8P, 3664-60-6P, 7-Octen-2-one
3710-30-3P, 1,7-Octadiene 3779-61-1P, 4065-80-9P, 4086-34-8P,
3-Cyclohexen-1-one 4187-81-9P, 4734-90-1P, 3-Cycloocten-1-one
5428-09-1P, 5558-87-2P, 5629-57-2P, 5666-17-1P, 6052-63-7P
6610-11-5P, 6-Methyl-2-cyclohexen-1-one 6728-26-3P,
(E)-Hex-2-enal 7065-05-6P, 7688-51-9P, 10006-38-9P
10281-55-7P, 10281-56-8P, 10428-96-3P, 10491-63-1P
10500-10-4P, 10500-11-5P, 10521-97-8P, 5-Phenylpent-3-en-2-one
12012-87-2P, Bis[(μ-chloro)(η³-2-chloroallyl)palladium]
12080-98-7P, 12084-71-6P, Bis[μ-acetato]bis(η³-
allyl)dipalladium 12090-04-9P, 12090-09-4P, 12090-69-6P
12097-84-6P, (η³-Allyl)chloro(triphenylphosphine)palladium
12099-33-1P, 12111-41-0P, 12129-99-6P, 12131-44-1P,
Bis[(μ-chloro)(η³-1-phenylallyl)palladium] 12145-53-8P
12154-16-4P, 12156-09-1P, 12182-26-2P, 12240-87-8P,
Bis[(η³-allyl)palladium] 12245-05-5P, 12245-22-6P
12245-27-1P, 12245-28-2P, 12245-51-1P, 12245-52-6P
12245-53-3P, 12245-70-4P, 12246-02-5P, 12281-94-6P
12288-41-4P, 12301-06-3P, 12302-54-4P, 12308-56-4P
12309-85-2P, 12395-90-4P, 13891-96-8P, 1-Undecen-1-ol
14320-37-7P, Cyclopent-3-en-1-one 14543-49-8P, 14815-73-7P
14815-74-8P, 15232-96-9P, 15874-80-3P, 16178-87-3P
16215-11-5P, 16424-35-4P, 16515-85-8P, 16717-84-3P
16818-61-4P, 18045-02-4P, 18355-70-9P, 18956-05-3P
19043-46-0P, 19752-23-9P, 20068-10-4P, (E)-4-Phenyl-3-
butenitrile 20202-62-4P, 20230-16-4P, 20337-93-9P
20461-31-8P, 21473-05-2P, 21488-83-5P, (Z)-1-Phenyl-3,7-
dimethylocta-2,6-diene 21677-96-3P, 21860-49-1P, 25554-22-1P
25859-52-3P, Methyl 3-methyl-3-butenolate 26450-24-8P
26462-12-3P, 26561-31-9P, 26561-32-0P, 26828-48-8P
27829-72-3P, 28973-98-0P, 29085-37-8P, 29330-76-5P
29330-77-6P, 29330-86-7P, 29330-86-7P, 30463-72-5P,
31666-74-7P, 31666-77-0P, 31985-02-1P, 32064-72-5P,

2-nonen-4-one 3267-81-9P 32715-98-3P 32732-73-3P
 32876-08-7P 32915-63-2P 32965-48-3P 33155-42-9P
 33379-48-5P 33584-32-3P 33596-78-2P 36321-95-6P
 36351-77-6P 36510-65-3P 36572-87-9P 36971-14-9P,
 1-Decen-4-ol 37464-41-8P 37575-80-7P 38282-07-4P
 38342-40-4P 38342-41-5P 40637-56-7P 40695-04-3P
 41348-25-8P 41449-89-4P 41557-81-7P 41562-41-8P
 41656-05-7P 42762-56-1P 42998-16-3P 49676-93-9P
 50404-95-0P 50487-71-3P 50507-72-7P 50994-84-8P
 51042-92-3P 51106-45-7P 51106-47-9P 51106-50-4P
 51106-51-5P 51106-53-7P 51106-54-8P 51729-84-1P
 52389-75-0P 52922-10-8P 52922-19-7P 53254-60-7P
 53265-48-8P 54162-19-5P 54340-71-5P 54829-97-9P
 54829-98-0P 54897-36-8P 54962-87-7P 55053-65-1P
 5512-78-7P, 1-Eicosen-3-one 55454-04-1P 55613-91-5P
 55684-63-4P 55903-11-2P 56084-53-8P 56505-44-3P
 57321-30-3P 57981-18-7P 58355-66-1P 58482-97-6P
 58527-00-7P 59053-07-1P 60038-55-3P 60410-18-6P
 60729-61-5P 60729-63-7P 61113-02-8P 61113-03-9P
 61113-04-0P 61128-77-6P 61168-10-3P, 1-Nonen-4-one
 61342-31-2P 61342-31-2P 61761-21-5P
 61874-40-4P 61305-24-6P 62015-29-5P 62075-33-6P
 61929-77-9P 63812-05-5P 63817-37-8P 62713-56-8P
 63138-98-7P 65280-46-8P 65337-70-4P 64841-68-5P
 65178-51-0P 67393-58-2P 67450-36-6P 65629-73-4P
 67099-84-7P 67393-58-2P 67450-36-6P 67463-14-3P
 67579-06-5P 68284-22-0P 68340-12-5P 67883-63-0P
 68276-71-1P 68284-22-0P 68340-12-5P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (Preparation and application of palladium-allyl complexes)
 THERE ARE 379 CITED REFERENCES AVAILABLE
 FOR THIS RECORD. ALL CITATIONS AVAILABLE
 IN THE RE FORMAT

L74 ANSWER 29 OF 67 HCAPLUS COPYRIGHT 2007 ACS ON STN
 ACCESSION NUMBER: 2003:169267 HCAPLUS Full-text
 DOCUMENT NUMBER: 139.353491
 TITLE: UK Speciated VOC emission inventories
 AUTHOR(S): Passant, N.; Woodfield, M.; Hayman, G.
 AEA Technology, National Environmental
 Technology Centre, Abingdon, UK
 CORPORATE SOURCE: Troposphere and Chemical Transformation in the
 Troposphere, Proceedings of EUROTRAC
 Symposium, 7th, Garmisch-Partenkirchen,
 Germany, Mar. 11-15, 2002 (2002),
 89-96. Editor(s): Midgley, Pauline M.;
 Reuther, Markus. Margraf Verlag: Welkerheim,
 Germany.
 CODEN: 69DQJ7; ISBN: 3-8236-1385-5
 Conference; (computer optical disk)
 DOCUMENT TYPE: English
 LANGUAGE: English
 ED Entered STN: 06 Mar 2003
 AB Volatile organic compounds (VOC), together with NOx lead to formation of ground-level O3.
 Over the past 10 yr, the UK has prepared speciated emission inventories of VOC to
 support the development of policies to control ground-level O3 formation. Preparation
 of a speciated VOC emission inventory is described and issues raised in its preparation
 and its subsequent validation against ambient hydrocarbon measurements are discussed.
 IT 78-79-5, Isoprene, reactions 79-20-9,
 Methylacetate 123-66-4, Butyl acetate 141-78-6
 , Ethyl acetate, reactions
 RL: OCU (Occurrence, unclassified); POL (Pollutant); RCT
 (Reactant); OCCU (Occurrence); RACT (Reactant or reagent)
 (ground-level ozone formation in relation to speciated volatile
 organic compound emission inventory in UK)
 RN 78-79-5 HCAPLUS
 CN 1,3-Butadiene, 2-methyl- (CA INDEX NAME)

CH3-C(=O)-CH=CH-CH3
 RN 79-20-9 HCAPLUS
 CN Acetic acid, methyl ester (CA INDEX NAME)

CH3-C(=O)-CH3
 RN 123-86-4 HCAPLUS
 CN Acetic acid, butyl ester (CA INDEX NAME)

CH3-C(=O)-CH2-CH3
 RN 141-78-6 HCAPLUS
 CN Acetic acid ethyl ester (CA INDEX NAME)

CH3-C(=O)-CH2-CH2-CH3
 Et-O-Ac

CC 59-2 (Air Pollution and Industrial Hygiene)
 IT Alcohols, reactions
 Aldehydes, reactions
 Alkanes, reactions
 Alkenes, reactions
 Alkynes
 Aromatic hydrocarbons, reactions
 Bsters, reactions
 Hydrocarbons, reactions
 Ketones, reactions
 Volatile organic compounds
 RL: OCU (Occurrence, unclassified); POL (Pollutant); RCT
 (Reactant); OCCU (Occurrence); RACT (Reactant or reagent)
 (ground-level ozone formation in relation to speciated volatile
 organic compound emission inventory in UK)
 IT 64-11-5, Ethanol, reactions 67-56-1, Methanol, reactions
 67-61-0, 2-Propanol, reactions 67-64-1, Acetone, reactions
 68-12-2, Dimethylformamide, reactions 71-26-3, 1-Butanol,
 reactions 71-43-2, Benzene, reactions 74-84-0, Ethane,
 reactions 74-85-1, Ethylene, reactions 74-87-3, Chloromethane,
 reactions 74-96-6, Propane, reactions 75-00-3, Chloroethane,
 reactions 75-09-2, Dichloromethane,
 reactions 75-28-5, Isobutane 75-35-4, 1,1-Dichloroethene,
 reactions 76-78-4, Isopentane 78-79-5, Isoprene,
 reactions 78-83-1, 2-Methyl-1-propanol, reactions 78-93-3,
 2-Butanone, reactions 79-01-6, Trichloroethene, reactions
 79-10-7, Acrylic acid, reactions 79-20-9, Methylacetate
 95-47-6, o-Xylene, reactions 96-14-0, 3-Methylpentane
 100-41-4, Ethylbenzene, reactions 106-42-3, p-Xylene, reactions
 106-97-8, Butane, reactions 106-98-9, 1-Butene, reactions

106-99-0, 1,3-Butadiene, reactions 107-06-2, 1,2-Dichloroethane, reactions 107-83-5, 2-Methylpentane 108-10-1, 4-Methyl-2-pentanone 108-38-3, m-Xylene, reactions 108-65-6, 1-Methoxy-2-propylacetate 108-88-3, Toluene, reactions 109-66-0, Benzene, reactions 110-54-3, Hexane, reactions 111-76-2, 2-Butoxyethanol 115-07-1, Propylene, reactions 115-10-6, Dimethylether 123-86-4, Butyl acetate 141-78-6, Ethyl acetate, reactions 142-82-5, n-Heptane, reactions 590-18-1, cis-2-Butene 624-64-6, trans-2-Butene 627-20-3, cis-2-Pentene 646-04-8, trans-2-Pentene 7397-62-8, Butyl glycolate 7446-09-5, Sulfur dioxide, reactions 7664-41-7, Ammonia, reactions 1104-93-1, Nitrogen oxide, reactions

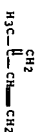
RL: OCC (Occurrence, unclassified); POL (Pollutant); RCT (Reactant); OCCU (Occurrence); RACT (Reactant or reagent) (ground-level ozone formation in relation to specified volatile organic compound emission inventory in UK)

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

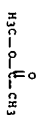
L74 ANSWER 30 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2001:808833 HCAPLUS Full-Text
 DOCUMENT NUMBER: 136:155317
 TITLE: Characterization of the reactivities of volatile organic compounds using a master chemical mechanism
 AUTHOR(S): Derwent, Richard G.; Jenkin, Michael E.; Saunders, Sandra M.; Pilling, Michael J.
 CORPORATE SOURCE: Climate Research Division, Meteorological Office, Bracknell, UK
 SOURCE: Journal of the Air & Waste Management Association (2001), 51(6), 699-707
 CODEN: JAWAFC; ISSN: 1096-2247
 PUBLISHER: Air & Waste Management Association
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 ED Entered STN: 07 Nov 2001

AB A comprehensive description of the O₃-forming potential of 101 organic compds. was developed under North American urban averaged conditions using a detailed master chemical mechanism and a simple air parcel trajectory model. This chemical mechanism describes reactions of 3603 chemical species occurring in >10,500 chemical reactions. An index value, calculated for each organic compound, describes the increment in O₃ concentration observed downwind from an urban area following emission of a fixed increment in the mass emission of each organic compound. These indexes, termed photochem. O₃ creation potentials (POCP), were expressed on a scale relative to ethylene (ethene) = 100; a reactivity scale was generated for alkenes, alkenes, and oxygenated and halogenated organic compds. A high degree of correlation (R² = 0.9) was observed between these POCP values and the most widely accepted urban reactivity scale. While reactivity of most of the 86 organic compds. compared fell within a consistent range, significant discrepancies were noted for only 5 compds. Single- or multi-day conditions appeared important in establishing quant. reactivity scales for less reactive organic compds.

IT 78-79-5, Isoprene, reactions 79-20-9, Methyl acetate 107-31-3, Methyl formate 108-21-4, Isopropylacetate 109-60-4, n-Propylacetate 123-86-4, n-Butylacetate 141-78-6, Ethyl acetate, reactions 540-88-5, tert-Butylacetate
 RL: POL (Pollutant); RCT (Reactant); OCCU (Occurrence); RACT (Reactant or reagent)
 (master chemical mechanism model to characterize atmospheric reactivity of volatile organic compds. and their ozone formation potential under North American urban average conditions)
 RN 78-79-5 HCAPLUS
 CN 1,3-Butadiene, 2-methyl- (CA INDEX NAME)



RN 79-20-9 HCAPLUS
 CN Acetic acid, methyl ester (CA INDEX NAME)



RN 107-31-3 HCAPLUS
 CN Formic acid, methyl ester (CA INDEX NAME)



RN 108-21-4 HCAPLUS
 CN Acetic acid, 1-methylethyl ester (CA INDEX NAME)



RN 109-60-4 HCAPLUS
 CN Acetic acid, propyl ester (CA INDEX NAME)



RN 123-86-4 HCAPLUS
 CN Acetic acid, butyl ester (CA INDEX NAME)



RN 141-78-6 HCAPLUS
 CN Acetic acid ethyl ester (CA INDEX NAME)



RN 540-88-5 HCAPLUS
 CN Acetic acid, 1,1-dimethylethyl ester (CA INDEX NAME)

CC

Section cross-reference(s): 53

59-2 (Air Pollution and Industrial Hygiene)
 50-00-0, Formaldehyde, reactions 57-55-6, Propylene glycol, reactions 60-29-7, Diethylether, reactions 64-17-5, Ethyl alcohol, reactions 64-18-6, Formic acid, reactions 64-19-7, Acetic acid, reactions 67-56-1, Methyl alcohol, reactions 67-63-0, Isopropanol, reactions 71-23-8, n-Propanol, reactions 71-36-3, Chloroform, reactions 71-55-6, Methyl chloroform 74-84-0, Ethane, reactions 74-85-1, Ethylene, reactions 74-87-3, Methyl chloride, reactions 74-98-6, Propane, reactions 75-07-0, Acetaldehyde, reactions 75-09-2, Methylene chloride, reactions 75-28-5, Isobutane 75-65-0, tert-Butanol, reactions 75-83-2, 2,2-Dimethylbutane 75-85-4, 2-Methyl-2-butanol 75-97-8, Methyl-tert-butylketone 78-78-4, Isopentane 78-79-5, Isoprene, reactions 78-83-1, Isobutanol, reactions 78-84-2, Isobutylaldehyde 78-92-2, sec-Butanol 78-93-3, Methylisobutylketone, reactions 79-01-6, Trichloroethylene, reactions 79-09-4, Propionic acid, reactions 79-20-9, Methyl acetate 79-29-8, 2,3-Dimethylbutane 80-56-8, a-Pinene 96-14-0, 3-Methylpentane 96-22-0, Diethylketone 105-46-4, sec-Butylacetate 106-97-8, n-Butane, reactions 106-98-9, But-1-ene, reactions 106-99-0, 1,3-Butadiene, reactions 107-21-1, Ethylene glycol, reactions 107-31-3, Methyl formate 107-83-5, 2-Methylpentane 107-87-9, Methylpropylketone 107-98-2, 1-Methoxy-2-propanol 108-10-1, Methylisobutylketone 108-20-3, Diisopropylether 108-21-4, Isopropylacetate 108-93-0, Cyclohexanol, reactions 108-94-1, Cyclohexanone, reactions 109-60-4, n-Propylacetate 109-66-0, n-Pentane, reactions 109-67-1, Pent-1-ene 109-86-4, 2-Methoxyethanol 110-55-3, n-Heptane, reactions 110-62-3, Valeraldehyde 110-80-3, 2-Ethoxyethanol 110-82-7, Cyclohexane, reactions 111-65-9, n-Octane, reactions 111-76-2, 2-Butoxyethanol 111-84-2, n-Nonane 112-40-3, n-Dodecane 115-07-1, Propylene, reactions 115-10-6, Dimethylether 123-38-6, Propionaldehyde, reactions 123-42-2, Diacetone alcohol 123-51-3, 3-Methyl-1-butanol 123-72-8, Butylaldehyde 123-86-4, n-Butylacetate 124-18-5, n-Decane 127-18-4, Tetrachloroethylene, reactions 137-32-6, 2-Methyl-1-butanol 141-78-6, Ethyl acetate, reactions 142-82-5, n-Heptane, reactions 156-59-2, cis-Dichloroethylene 156-60-5, 4-Ethyl-1-pentene 156-82-1, 2-Methylbut-2-ene 540-88-5, tert-Butylacetate 563-45-1, 3-Methylbut-1-ene 563-46-2, 2-Methylbut-1-ene 563-80-4, Methylisopropylketone 584-02-1, 3-Pentanol 589-34-4, 3-Methylhexane 589-38-8, Hexan-3-one 590-18-1, cis-But-2-ene 591-76-4, 2-Methylhexane 591-78-6, Hexan-2-one 592-41-6, Hex-1-ene, reactions 598-75-4, 3-Methyl-2-butanol 624-64-6, trans-But-2-ene 627-20-3, cis-Pent-2-ene 637-92-3, Ethyl-tert-butylether 646-04-8, trans-Pent-2-ene 1120-21-4, n-Undecane 1634-04-4, Methyl-tert-butylether 2278-22-0, Peroxyacetyl nitrate 4050-45-7, trans-Hex-2-ene 5131-66-8, 1-Butoxy-2-propanol 7688-21-3, cis-Hex-2-ene 7697-37-2, Nitric acid, reactions 10102-43-9, Nitric oxide, reactions 10102-44-0, Nitrogen dioxide, reactions 11104-93-1, Nitrogen oxide, reactions 25167-67-3, Butylene
 RL: POL (Pollutant); RCT (Reactant); OCCU (Occurrence); RACT (Reactant or reagent)
 (master chemical mechanism model to characterize atmospheric reactivity of volatile organic compds. and their ozone formation potential)

under North American urban average conditions)
 REFERENCE COUNT: 44
 THERE ARE 44 CITED REFERENCES AVAILABLE
 FOR THIS RECORD. ALL CITATIONS AVAILABLE
 IN THE RE FORMAT

174 ANSWER 31 OF 67 HCAPUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2001:143406 HCAPUS FULL-TEXT
 DOCUMENT NUMBER: 134:270429
 TITLE: Prediction of flammability of gases by using F-number analysis
 AUTHOR(S): Kondo, S.; Umano, Y.; Tokunashi, K.; Takahashi, A.; Tanaka, K.
 CORPORATE SOURCE: Research Institute of Innovative Technology for the Earth, National Institute of Materials and Chemical Research, Tsukuba, Ibaraki, 305-0046, Japan
 SOURCE: Journal of Hazardous Materials (2001 1, 82(2), 113-128
 CODEN: JHMA09; ISSN: 0304-3894
 Elsevier Science B.V.
 PUBLISHER: Journal
 LANGUAGE: English
 ED Entered STN: 28 Feb 2001
 AB A method of predicting flammability limits uses a flammability index called F-number for this purpose, an empirical expression of F-number was derived to account for the flammability characteristics of various organic substances. The anal. was done by fitting to the observed values of F-number for a wide variety of organic gases and vapors. F-number is an excellent tool to analyze the flammability characteristics of various substances. Upper and lower flammability limits can be derived from F-number together with the stoichiometric concentration collected for the effect of selective diffusion.

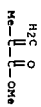
IT 78-79-5, Isoprene, reactions 79-20-9, Methylacetate 80-62-6, Methylmethacrylate 96-33-3, Methyl acrylate 96-34-4, Methyl chloroacetate 105-37-3, Ethylpropionate 107-31-3, Methyl formate 108-05-4, Vinyl acetate, reactions 108-21-4, Iso propylacetate 109-60-4, Propylacetate 109-94-4, Ethyl formate 110-19-0, Isobutyl acetate 110-49-6, Methyl cellosolve acetate 111-55-7, Glycol diacetate 123-86-4, Butyl acetate 123-82-2, Isobutyl acetate 140-88-5, Ethyl acrylate 141-32-2, Butylacrylate 141-78-6, Ethyl acetate, reactions 141-97-9, Ethyl acetoacetate 534-12-1, Methylpropionate 592-84-7, Butylformate 628-63-7, Amyl acetate
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (Prediction of flammability of gases by using F-number anal.)
 RN 78-79-5 HCAPUS
 CN 1,3-Butadiene, 2-methyl- (CA INDEX NAME)

CH₂
 $\text{H}_3\text{C}-\text{CH}=\text{CH}-\text{CH}_2$
 RN 79-20-9 HCAPUS
 CN Acetic acid, methyl ester (CA INDEX NAME)

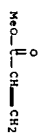
$\text{H}_3\text{C}-\text{C}(\text{O})-\text{CH}_3$

SN 10/564307 Page 79 of 139 STIC STN SEARCH 5/17/2007

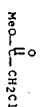
RN 80-62-6 HCAPLUS
CN 2-Propenoic acid, 2-methyl-, methyl ester (CA INDEX NAME)



RN 96-33-3 HCAPLUS
CN 2-Propenoic acid, methyl ester (CA INDEX NAME)



RN 96-34-4 HCAPLUS
CN Acetic acid, 2-chloro-, methyl ester (CA INDEX NAME)



RN 105-37-3 HCAPLUS
CN Propanoic acid, ethyl ester (CA INDEX NAME)



RN 107-31-3 HCAPLUS
CN Formic acid, methyl ester (CA INDEX NAME)



RN 108-05-4 HCAPLUS
CN Acetic acid ethenyl ester (CA INDEX NAME)



RN 108-21-4 HCAPLUS
CN Acetic acid, 1-methylethyl ester (CA INDEX NAME)

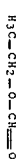
SN 10/564307 Page 80 of 139 STIC STN SEARCH 5/17/2007



RN 109-60-4 HCAPLUS
CN Acetic acid, propyl ester (CA INDEX NAME)



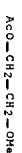
RN 109-94-4 HCAPLUS
CN Formic acid, ethyl ester (CA INDEX NAME)



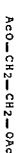
RN 110-19-0 HCAPLUS
CN Acetic acid, 2-methylpropyl ester (CA INDEX NAME)



RN 110-49-6 HCAPLUS
CN Ethanol, 2-methoxy-, 1-acetate (CA INDEX NAME)



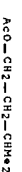
RN 111-59-7 HCAPLUS
CN 1,2-Ethanedithiol, 1,2-diacetate (CA INDEX NAME)



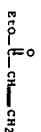
RN 123-86-4 HCAPLUS
CN Acetic acid, butyl ester (CA INDEX NAME)



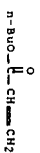
RN 123-92-2 HCAPLUS
CN 1-Butanol, 3-methyl-, 1-acetate (CA INDEX NAME)



RN 140-88-5 HCAPLUS
CN 2-Propenoic acid, ethyl ester (CA INDEX NAME)



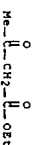
RN 141-32-2 HCAPLUS
CN 2-Propenoic acid, butyl ester (CA INDEX NAME)



RN 141-78-6 HCAPLUS
CN Acetic acid ethyl ester (CA INDEX NAME)



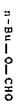
RN 141-97-9 HCAPLUS
CN Butanoic acid, 3-oxo-, ethyl ester (CA INDEX NAME)



RN 554-12-1 HCAPLUS
CN Propanoic acid, methyl ester (CA INDEX NAME)



RN 592-84-7 HCAPLUS
CN Formic acid, butyl ester (CA INDEX NAME)



RN 628-63-7 HCAPLUS
CN Acetic acid, pentyl ester (CA INDEX NAME)



CC 59-5 (Air Pollution and Industrial Hygiene)
IT 57-55-6, Propylene glycol, reactions 60-29-7, Ethylether, reactions 62-53-3, Aniline, reactions 64-17-5, Ethyl alcohol, reactions 64-19-7, Acetic acid, reactions 67-56-1, Methyl alcohol, reactions 67-63-0, Iso propyl alcohol, reactions 67-64-1, Acetone, reactions 71-23-8, Propyl alcohol, reactions 71-36-3, Butyl alcohol, reactions 71-41-0, Amyl alcohol, reactions 71-43-2, Benzole, reactions 71-55-6, 1,1,1-Trichloroethane 74-82-8, Methane, reactions 74-83-9, Methyl bromide, reactions 74-84-0, Ethane, reactions 74-85-1, Ethylene, reactions 74-86-2, Acetylene, reactions 74-87-3, Methyl chloride, reactions 74-89-5, Methylamine, reactions 74-96-4, Ethyl bromide 74-98-6, propane, reactions 75-00-3, Ethyl chloride 75-01-4, Vinylchloride, reactions 75-02-5, Vinylfluoride 75-04-7, Ethylamine, reactions 75-05-8, Acetonitrile, reactions 75-07-0, Acetaldehyde, reactions 75-09-2, Methylene chloride, reactions 75-10-5, Cyclopropane 75-21-8, Ethylene oxide, reactions 75-19-4, butane 75-29-6, Iso propyl chloride, reactions 75-28-5, Iso chloride, reactions 75-37-6, 1,1-Difluoroethane 75-38-7, Vinylidene fluoride 75-56-9, Propylene oxide, reactions 75-64-9, Tert butylamine, reactions 75-65-0, Tert butyl alcohol, reactions 75-68-3, 1-Chloro-1,1-difluoroethane 75-83-2, 2,2-Dimethylbutane 75-85-4, 2-Methyl-2-butanol 75-86-5, Acetone cyanohydrin 78-78-4, Isopentane 78-79-5, Isoprene, reactions 78-83-1, Iso butyl alcohol, reactions 78-84-2 78-87-5, Propylene dichloride 78-88-6, 2,3-Dichloropropene 78-92-2, 2-Butanol 78-94-4, Methyl vinyl ketone, reactions 79-01-6, Trichloroethylene, reactions 79-09-4, Propionic acid, reactions 79-10-7, Acrylic acid, reactions 79-20-9, Methylacetate 79-29-8, 2,3-Dimethylbutane 79-31-2, Iso butyric acid 79-46-9, 2-Nitropropane 80-62-6, Methylmethacrylate 85-44-9, Phthalic anhydride 91-20-3, Naphthalene, reactions 92-52-4, Biphenyl, reactions 95-47-6, o-Xylene, reactions 95-50-1, o-Dichlorobenzene 96-14-0, 3-Methylpentane 96-32-3, Methyl acrylate 96-34-4, Methyl chloroacetate 96-37-7, Methylcyclopentane 97-72-3, Isobutyric anhydride 97-96-1 97-99-4, Tetrahydrofurfuryl alcohol 98-00-0, Furfuryl alcohol 98-01-1, Furfural, reactions 98-06-6, Tert Butylbenzene 98-82-8, Cumene 100-41-4, Ethylbenzene, reactions 100-42-5, Styrene, reactions 103-09-3, 2-Ethylhexylacetate 103-65-1, Propylbenzene 104-51-8, Butylbenzene 104-76-7, 2-Ethylhexanol 105-05-5, p-Diethylbenzene 105-30-6 105-37-3, Ethylpropionate 105-46-4, Sec Butyl Acetate 105-57-7, Acetal 106-31-0, Butyric anhydride 106-42-3, p-Xylene, reactions 106-88-7, 1,2-Butylene oxide 106-89-8, Epichlorohydrin, reactions 106-95-6, Allyl bromide, reactions 106-97-8, Butane, reactions 106-98-9, 1-Butene, reactions 106-99-0, 1,3-Butadiene, reactions 107-02-8, Acrolein, reactions 107-05-1, Allyl chloride 107-06-2, Ethylene chloride, reactions 107-07-3, 2-Chloroethanol, reactions 107-10-8, Propylamine, reactions 107-11-9, Allylamine 107-13-1, Acrylonitrile, reactions 107-15-3, Ethylenediamine, reactions 107-18-6, Allyl alcohol, reactions 107-31-3, Methyl formate 107-83-5, Isohexane 107-87-9, Methylpropylketone 107-92-6, Butyric acid, reactions 108-05-4, Vinyl acetate, reactions 108-10-1, Methyl isobutyl ketone 108-11-2, Methyl isobutylcarbinol 108-18-9, Di-iso-propylamine 108-20-3, Isopropyl ether 108-21-4, Iso propylacetate 108-24-7, Acetic anhydride 108-31-6, Maleic anhydride, reactions 108-36-3, reactions

108-83-8, Di-isobutylketone 108-84-9, 108-87-2, 108-88-3, Di-isobutylketone 108-88-3, Toluol, reactions 108-90-7, Chlorobenzene, reactions 108-88-3, 108-94-1, Cyclohexanone, reactions 109-60-4, Propylacetate 109-65-9, Butyl bromide 109-69-3, 109-66-0, Pentane, reactions 109-67-1, 1-pentene 109-87-5, Butyl chloride 109-73-9, Butylamine, reactions 109-82-2, Vinyl ethyl ether 109-93-3, Divinyl ether 109-94-4, Ethyl formate 109-99-9, Tetrahydrofuran, reactions 110-00-9, Furan 110-12-3, Methylisobutylketone 110-19-0, Isobutyl acetate 110-43-0, Methylamylketone 110-49-6, Methyl cellosolve acetate 110-54-3, Hexane, reactions 110-58-7, Amylamine 110-82-7, Cyclohexane, reactions 110-88-3, Trioxane, reactions 110-91-8, Morpholine, reactions 111-40-0, Diethylene triamine 111-43-3, n-Propyl ether 111-55-7, Glycol diacetate 111-65-9, Octane, reactions 111-84-2, Nonane 112-27-6, Triethylene glycol 115-07-1, Propylene, reactions 115-10-6, Methyl ether 115-11-7, 2-Methylpropene, reactions 116-14-3, Tetrafluoroethylene, reactions 123-05-7, 2-Ethylhexanal 123-51-3, 123-20-6, Vinylbutyrate 123-62-6, Propionic anhydride 123-72-8, Butyl aldehyde 123-86-4, Butyl acetate 123-91-1, p-Dioxane, reactions 123-92-2, Isobutyl acetate 124-18-5, Decane 124-40-3, Dimethylamine, reactions 126-98-7, Methylacrylonitrile 126-99-8, 2-Chloro-1,3-butadiene 135-98-8, Sec Butylbenzene 140-88-5, Ethyl acrylate 141-32-2, Butylacrylate 141-78-6, Ethyl acetate, reactions 141-79-7, Mesityl oxide 141-97-9, Ethyl acetate 142-82-5, Heptane, reactions 142-96-1, Dibutyl ether 149-57-5, 2-Ethylhexanoic acid 151-56-4, Ethylamine, reactions 151-64-5, Cyclohexane 153-36-0, 1,1,2-Trifluoroethane 463-82-1, 2,2-Dimethylpropane 513-36-0, Iso butyl chloride 538-93-2, Isobutylbenzene 540-67-0, Propyl chloride 540-59-0, 1,2-Dichloroethylene 540-67-0, Methyl ethyl ether 542-55-2, Iso butylformate 542-75-6, 1,3-Dichloropropene 554-12-1, Methylpropionate 563-45-1, 3-Methyl-1-butene 563-47-3, Methyllyl chloride 564-02-3, 2,2,3-Trimethylpentane 565-59-3, 2,3-Dimethylpentane 584-02-1, 3-Pentanol 589-38-8, 3-Hexanone 590-18-1, cis-2-Butene 590-21-6, 1-Chloropropylene 591-97-9, 592-45-0, 1,4-Hexadiene 592-84-7, Butylformate 593-53-3, Methyl fluoride 593-60-2, Vinylbromide 593-70-4, Chlorofluoromethane 594-36-5, Tert Amyl chloride 624-64-6, trans-2-Butene 627-27-0, 3-Buten-1-ol 628-12-0, Ethylpropyl ether 628-63-7, Amyl acetate 821-55-6, Methylheptylketone 1067-20-5, 3,3-Diethylpentane 1321-74-0, Divinylbenzene, reactions 1331-43-7, Diethylcyclohexane 1640-88-7, Ethylcyclopentane 1653-19-6, 2,3-Dichlorobutadiene-1,3 1678-91-7, Ethylcyclohexane 1717-00-6, 1-Fluoro-1,1-dichloroethane 3266-23-7, 2,3-Butylene oxide 4170-30-3, Crotonaldehyde 4461-41-0, 2-Chloro-2-butene 4784-77-4, Crotyl bromide 4806-61-5, Ethylcyclobutane 6117-91-5, Crotonyl alcohol 7154-79-2, 2,2,3,3-Tetramethylpentane 12002-48-1, Trichlorobenzene 25013-15-4, Vinyltoluene 25167-70-8, 2,2,4-Trimethylpentane 25551-13-7, Trimethylbenzene 25567-67-3, Dinitrochlorobenzene 26519-91-5, Methylcyclopentadiene 26635-63-2, Sec Amyl alcohol 31394-54-4, Isobutane 62309-51-7, Propanol 80466-34-8, 2,4-Hexadienal RN: RCT (Reactant); RACT (Reactant or reagent)

REFERENCE COUNT: 7

7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

TITLE: POCP for individual VOC under European conditions

AUTHOR(S): Altenstedt, Johannes; Pleijel, Karin

CORPORATE SOURCE: Göteborg, Swed.

SOURCE: IVL Report (1998), B 1305, 1-47

DOCUMENT TYPE: Report

LANGUAGE: English

AB: Entered STN: 11 Jan 1999

03 production from volatile organic compds. (VOC) in the atmospheric is discussed, focusing on a general way to present photochem. O3 creation potential (POCP) values for different VOC under European conditions and to calculate such values for a large number of VOC. Topics discussed include: environmental impact of VOC in atmospheric tropospheric O3; the photo-stationary state; NOx and VOC precursors of tropospheric O3; atmospheric chemical of VOC; ranking VOC according to their ability to produce O3; methods for critical anal. of POCP concept; results from critical anal. of the POCP concept; selecting model set-up to calculate POCP; POCP under European conditions; and conclusions.

IT 78-79-5, Isoprene, reactions 79-20-9, Methylacetate 123-86-4, n-Butylacetate 141-78-6, Ethylacetate, reactions 141-79-7, RLT: POL (Pollutant); RCT (Reactant); OCCU (Occurrence); RACT (Reactant or reagent) (modelling photochem. ozone creation potentials and air pollution for individual volatile organic compds. in troposphere of Europe)

RN 78-79-5, HCAPLUS

CN 1,3-Butadiene, 2-methyl- (CA INDEX NAME)

H3C-CH=CH-CH2

RN 79-20-9, HCAPLUS

CN Acetic acid, methyl ester (CA INDEX NAME)

H3C-C(=O)-CH3

RN 123-86-4, HCAPLUS

CN Acetic acid, butyl ester (CA INDEX NAME)

n-Bu-C(=O)-Ac

RN 141-78-6, HCAPLUS

CN Acetic acid ethyl ester (CA INDEX NAME)

Et-C(=O)-Ac

CC 59-2 (Air Pollution and Industrial Hygiene)

(modeling photochem. ozone creation potentials and air pollution for individual volatile organic compds. in troposphere of Europe)

50-00-0, formaldehyde, reactions 60-29-1, Diethyl ether, reactions 64-17-5, Ethanol, reactions 64-19-7, Acetic acid, reactions 67-56-1, Methanol, reactions 67-63-0, Isopropanol, reactions 67-64-1, Acetone, reactions 71-36-3, n-Butanol, reactions 71-33-2, Benzene, reactions 71-55-6, 1,1-Trichloroethane 74-82-8, Methane, reactions 74-84-0, Ethane, reactions 74-85-1, Ethene, reactions 74-86-2, Acetylene, reactions 74-93-1, Methyl mercaptan, reactions 74-98-6, Propane, reactions 75-07-0, Acetaldehyde, reactions 75-18-3, Dimethyl sulfide 75-28-5, Iso-butane 75-34-3, 1,1-Dichloroethane 75-35-4, 1,1-Dichloroethane, reactions 78-78-4, Isopentane 78-79-5, Isoprene, reactions 78-84-2, Isobutyraldehyde 78-85-3, Methacrolein 78-93-3, Ethyl methyl ketone, reactions 78-98-8, Methylglyoxal 79-01-6, Trichloroethene, reactions 79-20-9, Methylacetate 95-47-6, o-Xylene, reactions 95-63-6, 1,2,4-Trimehybenzene 96-14-1, 3-Methylpentane 98-82-8, Isopropylbenzene 100-41-4, Ethylbenzene, reactions 100-42-5, Styrene, reactions 100-52-7, Benzaldehyde, reactions 103-65-1, n-Propylbenzene 105-66-4, sec-Butylacetate 106-42-3, p-Xylene, reactions 106-97-8, Butene, reactions 106-98-9, 1-Butene, reactions 107-01-7, 2-Butene 107-02-8, Acrolein, reactions 107-06-2, 1,2-Dichloroethane, reactions 107-22-2, Glyoxal 107-83-5, Methylpentane 108-10-1, Methyl isobutyl ketone 108-38-3, m-Xylene, reactions 108-67-8, 1,3,5-Trimethylbenzene, reactions 108-67-2, Methylcyclohexane 108-88-3, Toluene, reactions 109-66-0, Pentane, reactions 109-67-1, 1-Pentene 109-66-2, 2-Pentene 110-34-3, Hexane, reactions 110-62-3, Valeraldehyde 111-65-9, Octene, reactions 111-84-2, Nonane 112-40-3, Dodecane 115-07-1, Propene, reactions 123-38-6, Propionaldehyde, reactions 123-77-8, Butyraldehyde 123-66-4, n-Butylacetate 124-18-5, Decane 127-18-4, 1,2-Trichloroethene, reactions 141-78-6, Ethylacetate, reactions 142-82-5, Heptane, reactions 513-35-9, 2-Methyl-2-butene 526-73-8, 1,2,3-Trimehybenzene 563-66-2, 2-Methyl-1-butene 592-72-8, 2-Methylheptane 611-14-3, o-Ethyltoluene 620-94-4, m-Ethyltoluene 622-96-6, p-Ethyltoluene 624-92-0, Dimethyl disulfide 630-08-0, Carbon monoxide, reactions 871-83-0, 2-Methylnonane 1120-21-4, Undecane 1534-04-4, Methyl tertbutylamine 3221-61-2, 2-Methyloctane 6975-98-0, 2-Methyldecane R.I. POL (POLUTANT); RCT (Reactant); OCCU (Occurrence); RACT (Reactant or Reagent)

(modeling photochem. ozone creation potentials and air pollution for individual volatile organic compds. in troposphere of Europe)

42 THERE ARE 42 CITED REFERENCES AVAILABLE

17(1), 16-20
CODEN: LHYGD7; ISSN: 0253-2417
Linchan Huaxue Yu Gongye Bianji Weiyuanhui

DOCUMENT TYPE: Journal
LANGUAGE: Chinese
ED: 1949-1954

The esterification of linallyl, geranyl and neryl chlorides with NaOAc was studied. The effects of catalysts, reaction temperature and the comp. of hydrochloralides on the distribution of esters were investigated in detail. Results showed that all three allyl-type chlorides can be esterified with sodium acetate in acetic acid to yield linallyl acetate with 96% or more selectively when catalyzed by CuCl₂. In the presence of Et₃N, the three allyl-type chlorides were converted to their acetates resp. linallyl acetate can be obtained with 96.58% selectively under the optimum conditions.

11	1,2,3-5-3, myricene 1,21-09-3, sodium acetate
	RT: RCT (Reactant); RACT (Reactant or reagent)
	(cupric chloride catalyzed hydrochlorination of myricene and
	esterification of alkyl-type chlorides)
RN	123-35-3 HCAPLUS
CN	1,6-Octadiene, 7-methyl-3-methylene- (CA INDEX NAME)

RN	127-09-3	HCAPLUS
CN	Acetic acid, sodium salt (1:1)	(CA INDEX NAME

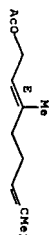


IT 105-87-97, Gemanyl acetate 135-95-9P, linallyl acetate 141-13-8P, Neryl 135-96-9P, R.I. SPCN (Synthetic Preparation); PMP (Preparation) (cupric chloride catalyzed hydrochlorination of myrcene and esterification of alkyl-type chlorides)

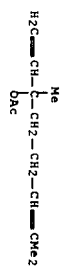
RM 105-87-5 HCAPUS

CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (ZE) - (CA INDEX NAME)

Double bond geometry as shown.

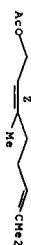


RN 115-95-7 HCAPLUS
CN 1,6-Octadien-3-ol, 3,7-dimethyl-, 3-acetate (CA INDEX NAME)



RN 141-12-8 HCAPLUS
CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2Z) - (CA INDEX NAME)

Double bond geometry as shown.



CC 30-10 (Terpenes and Terpenoids)
IT 123-35-3, Myrcene 127-09-3, Sodium acetate
471-10-3, Linalyl chloride 5389-87-7, Geranyl chloride
20536-36-1, Neryl chloride

RL: RCT (Reactant); RACT (Reactant or reagent)

(cupric chloride catalyzed hydrochlorination of myrcene and esterification of alkyl-type chlorides)
IT 105-87-3P, Geranyl acetate 115-95-7P, Linalyl acetate 141-12-8P, Neryl acetate

RL: SPN (Synthetic preparation); PREP (Preparation)
(cupric chloride catalyzed hydrochlorination of myrcene and esterification of alkyl-type chlorides)

L74 ANSWER 34 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1997:62046 HCAPLUS Full-text
DOCUMENT NUMBER: 126:157642
TITLE: Research and development in synthesis of series fine chemicals from rosin and turpentine. IV. Synthesis of neryl and geranyl acetates

AUTHOR(S): Li, Qianhe; Yin, Dulin; Li, Haotao; Lin, Liden; Ma, Runei

CORPORATE SOURCE: Institute of Fine Catalysts and Synthesis, Hunan Teacher's University, Changsha, 410081, Peop. Rep. China

SOURCE: Hunan Shifan Daxue Zixun Kexue Xuebao (1996), 19(3), 34-37

PUBLISHER: CODEN: HSDXEL; ISSN: 1000-2537

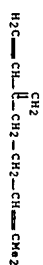
DOCUMENT TYPE: Journal

LANGUAGE: Chinese

ED Entered STN: 29 Jan 1997
AB Neryl and geranyl acetates were synthesized from β -pinene in turpentine oil by a 3-step process consisting of catalytic isomerization, hydrochlorination, and esterification. The effect of the esterification conditions on the yield of the title compds. was studied. In the presence of 28 Et3N (the catalyst) myrcene hydrochlorination crude products reacted with equimolar anhydrous NaOAc at 85-90° for 5 h, the total yield of the 2 title esters reached 66.6% based on β -pinene, in which ester products the selectivity of neryl acetate was 40-45% whereas that of geranyl acetate was 55-60%.

IT 123-35-3DP, Myrcene, hydrochlorination products
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

RN 123-35-3 HCAPLUS
CN 1,6-Octadiene, 7-methyl-3-methylene- (CA INDEX NAME)



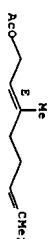
IT 105-87-3P, Geranyl acetate 141-12-8P, Neryl acetate

RL: SPN (Synthetic preparation); PREP (Preparation)

(β -pinene conversion to neryl acetate and geranyl acetate)
RN 105-87-3 HCAPLUS

CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2E) - (CA INDEX NAME)

Double bond geometry as shown.



RN 141-12-8 HCAPLUS
CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2Z) - (CA INDEX NAME)

Double bond geometry as shown.



CC 30-10 (Terpenes and Terpenoids)
IT 123-35-3DP, Myrcene, hydrochlorination products
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(β -pinene conversion to neryl acetate and geranyl acetate)
IT 105-87-3P, Geranyl acetate 141-12-8P, Neryl acetate

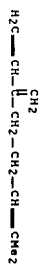
RL: SPN (Synthetic preparation); PREP (Preparation)
(β -pinene conversion to neryl acetate and geranyl acetate)

L74 ANSWER 35 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1995:741485 HCAPLUS Full-text
DOCUMENT NUMBER: 123:339558

TITLE: Tetraacyanoethylene-hydrogen peroxide, a mild

epoxidation system of olefins
AUTHOR(S): Masaki, Yukio; Miura, Tsuyoshi; Mukai, Isao; Iwata, Ichiro; Oda, Hirohisa; Itoh, Atsichika
Gifu Pharmaceutical Univ., Gifu, 502, Japan
CORPORATE SOURCE: Chemical & Pharmaceutical Bulletin (1995), 43(4), 686-8

PUBLISHER: CODEN: CEBPAL; ISSN: 0009-2363
Pharmaceutical Society of Japan



CC	30-1 (Terpenes and Terpenoids)
	Section cross-reference(s): 5, 22
IT	76-49-3, Bornyl acetate 79-92-5, Camphene 80-56-8,

Myrcene 1127-91, β -pinene 138-66, limonene 464-48-2, (1S)-(-)-Camphor 470-82-6, 1,8-Cineole 501-52-0, Hydrocinnamic acid 562-74-3, 4-Terpineol 1135-24-6, Furfic acid 1195-01-6, 2009-00-9, (+)-Sabinene 2244-16-8, (-)-Carvone 7764-60-9, 18486-69-6, (1R)-(-)-Myrcenal 1894-97-4, (1R)-(-)-Myrcenol 22567-21-1, 32719-61-2, Eucalyptone 113412-11-6, Calamanthone 113549-80-9, Desacetylcalamanthone

RT: RCT (Reactant), RACT (Reactant or reagent)

(water solubility of, determination of, via gas chromatog.)

L74 ANSWER 37 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STING
ACCESSION NUMBER: 1991:164539 HCAPLUS Full-text
DOCUMENT NUMBER: 114:164539
TITLE: Reductive radical cyclizations

AUTHOR(S) :

CORPORATE SOURCE:

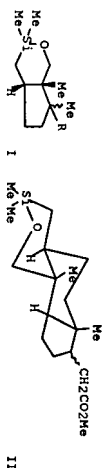
SOURCE: Helvetica Chimica Acta (1991),

74(1), 146-62

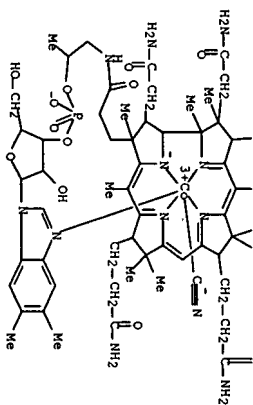
DOCUMENT TYPE:

OTHER SOURCE(S): CASREACT 114:164539

ED Entered STN: 03 May 1991



AB The tin hydride promoted and the reductive vitamin B12 catalyzed radical cyclization of mixed 2-bromoacetaldehyde acetals and of (2-bromoethyl)dimethylsilyl ethers of allylic/terpenoid alcs. was investigated: 3-oxodeca-5,9-dien-1-yl radicals undergo 5-exo-cyclization to oxolanes, 3-oxa-2-siladeca-5,9-dien-1-yl radicals sequential 6-endo-5-



PAGE 2-*p*

PAGE 1-A

IT	105-45-3, Methyl acetoacetate
	RL: RCT (Reactant); RACT (Reactant or reagent)
	(dication alkylation of, with silylgeranyl bromide)
RN	105-45-3 HCAPLUS
CN	Butanoic acid, 3-oxo-, methyl ester (CA INDEX NAME)

DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 123-339558
 ED Entered STN: 17 Aug 1995
 GI



II

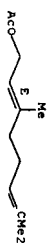
AB A reagent combination system, tetraacynoethylene (1)-30% H₂O₂, epoxidized olefins efficiently in MeCN at room temperature in a stereospecific manner with retention of the configuration of the double bond. H₂O₂ 30% was added to I and cis-3-hexen-1-ol in MeCN at room temperature for 12 h to give cis-II.
 IT 105-87-3 123-35-3 540-88-5, tert-Butyl acetate

RL: RCT (Reactant); RACT (Reactant or reagent)

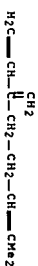
(tetraacynoethylene-hydrogen peroxide, a mild epoxidn. system of olefins)

RN 105-87-3 HCAPLUS
 CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



RN 123-35-3 HCAPLUS
 CN 1,6-Octadiene, 7-methyl-3-methylene- (CA INDEX NAME)



RN 540-88-5 HCAPLUS
 CN Acetic acid, 1,1-dimethylethyl ester (CA INDEX NAME)



CC 27-2 (Heterocyclic Compounds (One Hetero Atom))
 IT 105-87-3 106-23-0 106-24-1 108-98-5, Benzenethiol, reactions 110-93-0 123-35-3 540-88-5, tert-Butyl acetate 870-63-3, 1-Bromo-3-methyl-2-butene 928-96-1, cis-3-Hexen-1-ol 3695-38-3 42272-94-6 42602-37-9 5113-72-5 52188-73-5 76871-78-8 88191-39-3
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (tetraacynoethylene-hydrogen peroxide, a mild epoxidn. system of olefins)

174 ANSWER 36 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1994-8750 HCAPLUS Full-text
 DOCUMENT NUMBER: 120-8750
 TITLE: Just how insoluble are monoterpenes?
 AUTHOR(S): Weidenhamer, Jeffrey D.; Macias, Francisco A.; Fischer, Nikolaus H.; Williamson, G. Bruce
 CORPORATE SOURCE: Dep. Chem., Louisiana State Univ., Baton Rouge, La, 70803, USA
 SOURCE: Journal of Chemical Ecology (1993), 19(8), 1799-807
 CODEN: JCECD8; ISSN: 0098-0331

DOCUMENT TYPE: Journal

LANGUAGE: English

ED Entered STN: 08 Jan 1994

AB Prior generalizations about the ecol. roles of monoterpenes may be misleading if based on the presumed insol. of monoterpenes in water. The authors determined the aqueous solubility of 31 biol. active monoterpenes by gas chromatog. While hydrocarbons were of low solubility (<35 ppm), oxygenated monoterpenes exhibited solubilities one or two orders of magnitude higher, with ranges of 155-6990 ppm for ketones and of 183-1560 ppm for alcs. Many monoterpenes are phytotoxic in concns. under 100 ppm, well below the saturated aqueous concns. of oxygenated monoterpenes. Therefore, even dilute, unsatd. solns. of monoterpenes, occurring naturally in plant tissues and soil solns., may act as potent biol. inhibitors.

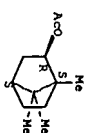
IT 76-49-3, Borneyl acetate 105-87-3, Geranyl acetate 115-95-7, Linalyl acetate 123-35-3, Myrcene

RL: RCT (Reactant); RACT (Reactant or reagent)

(water solubility of, determination of, via gas chromatog.)

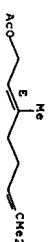
RN 76-49-3 HCAPLUS
 CN Bicyclo[2.2.1]heptan-2-ol, 1,7,7-trimethyl-, 2-acetate, (1R,2S,4R)-rel- (CA INDEX NAME)

Relative stereochemistry.

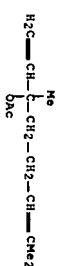


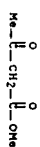
RN 105-87-3 HCAPLUS
 CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2E)- (CA INDEX NAME)

Double bond geometry as shown.

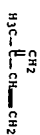


RN 115-95-7 HCAPLUS
 CN 1,6-Octadien-1-ol, 3,7-dimethyl-, 3-acetate (CA INDEX NAME)



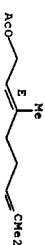


- IT 78-79-5, Isoprene, reactions
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (hydroxy bromination and epoxide formation of)
 RN 78-79-5 HCAPLUS
 CN 1,3-Butadiene, 2-methyl- (CA INDEX NAME)



- IT 105-87-3
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (oxidation of, with selenium dioxide)
 RN 105-87-3 HCAPLUS
 CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2E)- (CA INDEX NAME)

Double bond geometry as shown.

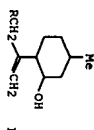


- CC 30-15 (Terpenes and Terpenoids)
 Section cross-reference(s): 26.
 IT 68-19-9, Vitamin B12
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (catalyst for reductive radical cyclization of terpenoid bromoacetate or bromomethylsilyl ether)
 IT 105-45-3, Methyl acetate
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (dianion alkylation of, with siloxysteranyl bromide)
 IT 78-79-5, Isoprene, reactions
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (hydroxy bromination and epoxide formation of)
 IT 105-87-3
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (oxidation of, with selenium dioxide)

L74 ANSWER 38 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1990:459553 HCAPLUS Full-text
 DOCUMENT NUMBER: 113:59553
 TITLE: Allylic chlorination of isoprene-type olefins
 with sulfuric chloride
 AUTHOR(S): Bolland, Michel; Balme, Genevieve; Gore, Jacques
 CORPORATE SOURCE: ESCIL, Univ. Claude Bernard, Villeurbanne, 69622, Fr.
 SOURCE: Tetrahedron Letters (1989), 30(42), 5767-70
 CODEN: TELENY; ISSN: 0040-4039
 DOCUMENT TYPE: Journal
 LANGUAGE: French

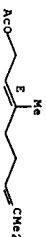
OTHER SOURCE(S): CASREACT 113:59553

ED Entered STN: 17 Aug 1990
 GI



- AB Sulfuryl chloride is a convenient reagent for the allylic chlorination of olefins bearing an isopropenyl or isopropylidenyl moiety. The substitution occurs with good yields and with allylic rearrangement, giving in most cases a secondary chloride. Thus, isopulegol (I, R = H) when tested with SOCl₂ at 0°, gave 71% chloride I (R = Cl).
 IT 105-87-3 123-35-3, Myrcene
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (regioselective allylic chlorination of)
 RN 105-87-3 HCAPLUS
 CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



- RN 123-35-3 HCAPLUS
 CN 1,6-Octadiene, 7-methyl-3-methylene- (CA INDEX NAME)

$$\text{H}_2\text{C}=\overset{\text{CH}_3}{\text{C}}-\text{CH}_2-\text{CH}_2-\text{CH}=\text{CH}_2$$

- CC 30-10 (Terpenes and Terpenoids)
 IT 78-70-6, Linalool 89-79-2, Isopulegol 105-87-3
 IT 106-24-1 123-35-3, Myrcene 556-82-1, Prenol 763-32-6, 3-Methyl-3-buten-1-ol 928-92-7 4057-42-5 6090-05-7 66312-97-3
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (regioselective allylic chlorination of)

L74 ANSWER 39 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1991:6833 HCAPLUS Full-text
 DOCUMENT NUMBER: 114:6833
 TITLE: Synthesis of geraniol and nerol
 AUTHOR(S): Liu, Xianzhong; Wang, Zhenhong; Jiang, Tongfu
 CORPORATE SOURCE: Res. Inst. Chem. Process, Util. For. Prod., Chin. Acad. For., Nanjing, Peop. Rep. China
 SOURCE: Linchen Huaxue Yu Gongye (1989), 9(4), 11-19
 CODEN: LINGDT; ISSN: 0253-2417
 DOCUMENT TYPE: Journal

LANGUAGE: Chinese

ED Entered STN: 12 Jan 1991

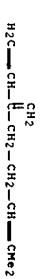
AB The synthetic route of geraniol and nerol was studied. Myrcene which was obtained from p-pine in gum turpentine by heat isomerization was used as raw material. In the presence of catalytic myrcene was treated by addition of HCl to form an adduct mixture consisting mainly of geranyl chloride and neryl chloride with small amounts of other chlorides such as linalyl chloride and turpene present. These then converted sep. to their resp. acetate esters by treatment with sodium acetate in the presence of a catalyst. The major products are geranyl acetate and neryl acetate. The yield of the acetates was 50-60%, and the ratio of geranyl acetate to neryl acetate in the mixed reaction time were investigated. Saponification of the acetates produced the resp. alcs. Pure geraniol and nerol were separated by rectification on a highly efficient packed column.

IT 123-35-3, Myrcene

RL: RCT (Reactant); RACT (Reactant or reagent)

CN 123-35-3 HCAPLUS

CN 1,6-Octadiene, 7-methyl-3-methylene- (CA INDEX NAME)



IT 105-87-3P, Geranyl acetate 141-12-8P, Neryl acetate

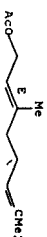
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(Preparation and saponification of)

CN 105-87-3 HCAPLUS

CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



RN 141-12-8 HCAPLUS
CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2Z)- (CA INDEX NAME)

Double bond geometry as shown.



CC 30-10 (Terpenes and Terpenoids)

IT 123-35-3, Myrcene

RL: RCT (Reactant); RACT (Reactant or reagent)

CN (Chlorination of)

IT 105-87-3P, Geranyl acetate 141-12-8P, Neryl acetate

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(Preparation and saponification of)

L74 ANSWER 40 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1989:439594 HCAPLUS Full-text

DOCUMENT NUMBER: 111:39594

TITLE: The regioselectivity of elimination reactions

AUTHOR(S):

CORPORATE SOURCE:

SOURCE:

DOCUMENT TYPE:

LANGUAGE:

OTHER SOURCE(S):

ED Entered STN: 05 Aug 1989

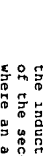
AB Tertiary alcs. with prenyl or geranyl moieties, bearing a second oxygen function in the 3, 4 or 5 position were dehydrated under various conditions: the composition of the olefinic mixture obtained was accounted for, by an intramol. base relay effect. Basic elimination of analogous dimethylsulfonium salts gave results that could be related to the inductive effect: a correlation between regioselectivity and the Taft constant of the second oxygen function was found, except for the very basic alkoxide groups where an alternative regioselective elimination took place.

IT 108-59-8, Dimethyl malonate

RL: RCT (Reactant); RACT (Reactant or reagent)

CN 108-59-8 HCAPLUS

CN Propanedioic acid, 1,3-dimethyl ester (CA INDEX NAME)



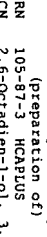
IT 105-87-3P 141-12-8P
RL: SPN (Synthetic preparation); PREP (Preparation)

(Preparation of)

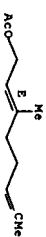
CN 105-87-3 HCAPLUS

CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



Double bond geometry as shown.

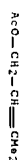


RN 141-12-8 HCAPLUS
CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2Z)- (CA INDEX NAME)

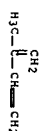
Double bond geometry as shown.



IT 1191-16-8P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (Preparation of, via dehydration of tertiary terpene alcs.)
 RN 1191-16-8 HCAPLUS
 CN 2-Buten-1-ol, 3-methyl-, 1-acetate (CA INDEX NAME)



IT 78-79-5, Isoprene, reactions
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (Reaction of, dimethylsulfide, sulfonium salt from)
 RN 78-79-5 HCAPLUS
 CN 1,3-Butadiene, 2-methyl-, (CA INDEX NAME)



CC 30-10 (Terpenes and Terpenoids)
 Section cross-reference(s): 22
 IT 108-59-8, Dimethyl malonate
 RL: RCT (Reactant); RACT (Reactant or reagent)

(alkylation of, by prenyl bromide or tosylate)
 IT 105-87-3P 106-24-1P 106-25-2P 141-12-8P
 459-88-1P 3239-35-8P 3239-37-0P 5944-20-7P 6819-18-1P
 7733-91-7P 13066-51-8P 20776-25-4P 27557-60-4P 40121-12-8P
 53840-11-2P 55039-75-3P 62947-42-6P 63343-20-4P
 69301-53-7P 69301-54-8P 71724-57-7P 72858-60-7P
 74380-61-3P 77958-38-4P 100669-16-7P 100669-17-8P
 107697-13-2P 107697-18-7P 107697-26-7P 107697-29-0P
 121402-99-1P 121403-00-7P 121403-01-8P 121403-02-9P
 121403-03-0P 121403-17-6P 121403-19-8P 121403-21-2P
 121403-22-3P 121403-23-4P 121403-26-7P 121403-27-8P
 121403-28-9P 121403-29-0P 121403-30-3P 121403-31-4P
 121403-32-5P 121403-33-6P 121403-34-7P 121403-35-8P
 121403-36-9P 121403-37-0P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (Preparation of)

IT 556-82-1P 763-89-3P 929-12-4P 1191-16-8P
 1569-60-4P 14309-15-0P 16993-86-5P 19162-00-6P 22094-02-6P
 35901-76-9P 88626-62-4P 88626-76-0P 88626-78-2P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (Preparation of, via denaturation of tertiary terpene alcs.)

IT 78-79-5, Isoprene, reactions
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (Reaction of, dimethylsulfide, sulfonium salt from)

L74 ANSWER 41 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1989-633218 HCAPLUS Full-text
 DOCUMENT NUMBER: 111:233218

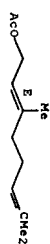
AUTHOR(S):
 ALLYLIC chlorination of isoprenoid
 oligoolefins with sulfur chloride
 Veselovskii, V. V.; Dzygan, V. A.; Gafurov, N.
 M.; Adenkov, S. M.; Kagaritskii, A. D.;
 Maksimov, B. I.; Chizhov, O. S.; Moiseenko,
 A. M.
 Inst. Org. Khim. im. Zelinskogo, Moscow, USSR
 Izvestiya Akademii Nauk SSSR, Seriya
 Khimicheskaya (1988), (10), 2423-4

DOCUMENT TYPE: CODEN: IASKA6; ISSN: 0002-3353
 LANGUAGE: Journal
 OTHER SOURCE(S): Russian
 CASREACT 111:233218

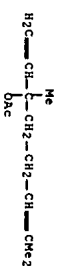
ED Entered STN: 23 Dec 1989
 AB ALLYLIC chlorination of Me2C:CHR [R = CH2CH2CHMeCH2CH2OAc, CH2CH2CHMe:CHCH2OAc, CH2CH2CHMe:CHCH2OAc, CH2CH2CHMe(OAc)CH:CH2] by SO2Cl2 in CH2Cl2 containing C5H5N gave 40-84% chlorides CH2:CHMeCHClR. The use of CH2Cl2 as a solvent instead of CCl4 decreases the yields of Me2C(Cl)CHClR to 52%.

IT 105-87-3 115-95-7 123-35-3
 141-12-8 150-84-5
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (Allylic chlorination of, by sulfur chloride)
 RN 105-87-3 HCAPLUS
 CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (12E)- (CA INDEX NAME)

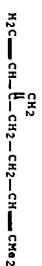
Double bond geometry as shown.



RN 115-95-7 HCAPLUS
 CN 1,6-Octadien-3-ol, 3,7-dimethyl-, 3-acetate (CA INDEX NAME)



RN 123-35-3 HCAPLUS
 CN 1,6-Octadiene, 7-methyl-3-methylene- (CA INDEX NAME)

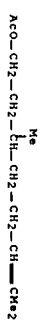


RN 141-12-8 HCAPLUS
 CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (12Z)- (CA INDEX NAME)

Double bond geometry as shown.



RN 150-84-5 HCAPLUS
 CN 6-Octen-1-ol, 3,7-dimethyl-, 1-acetate (CA INDEX NAME)



CC 30-10 (Terpenes and Terpenoids)
IT 105-87-3 115-95-7 123-35-3

141-12-8 150-84-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(allylic chlorination of, by sulfoxyl chloride)

174 ANSWER 42 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1989:534484 HCAPLUS Full-Text
DOCUMENT NUMBER: 111:134484

AUTHOR(S): Reaction of sulfoxide hydrochlorides and hydrobromides with trisubstituted olefins
Moiseenkov, A. M.; Dragan, V. A.; Lozanova, A. V.; Veselovskii, V. V.
CORPORATE SOURCE: Inst. Org. Khim. im. Zelinskogo, Moscow, USSR
Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya (1988), (8), 1797-803
CODEN: IASRA6; ISSN: 0002-3353

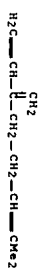
DOCUMENT TYPE: Journal

LANGUAGE: Russian

OTHER SOURCE(S): CASREACT 111:134484

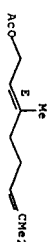
ED Entered STN: 14 Oct 1989
AB Chlorination of Me₂C=CHCH₂CH₂C(X)Me (X = H, OMe, H, CH₂CH₂OMe; CHCH₂OMe) by RI₂SO HCl (RI = Me, Ph, R₁₂ = (CH₂)₄) in MeNO₂ or CH₂Cl₂ containing CH₂Cl₂ or LiClO₄ or by Cl₂-CCl₄ at -50° or by HCl-AcOH at 0° gave mixts. containing CH₂C(Me)CHClCH₂CH₂C(X)Me, Me₂CCl(CH₂)₃C(X)Me, and Me₂CClCHClCH₂CH₂C(X)Me whose yields and ratios depended on the process. Addnl. obtained were some bromo derivs.

IT 123-35-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(bromination of)
RN 123-35-3 HCAPLUS
CN 1,6-Octadiene, 7-methyl-3-methylene- (CA INDEX NAME)

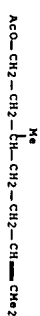


IT 105-87-3 150-84-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(chlorination and bromination of, by sulfoxide hydrochlorides and hydrobromides)
RN 105-87-3 HCAPLUS
CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



RN 150-84-5 HCAPLUS
CN 6-Octen-1-ol, 3,7-dimethyl-, 1-acetate (CA INDEX NAME)



CC 30-10 (Terpenes and Terpenoids)
IT 123-35-3

123-35-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(bromination of)

IT 105-87-3 150-84-5 19162-00-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(chlorination and bromination of, by sulfoxide hydrochlorides and hydrobromides)

174 ANSWER 43 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1988:493347 HCAPLUS Full-Text
DOCUMENT NUMBER: 109:93347

AUTHOR(S): Regiospecific ene-type reaction of benzenesulfinyl chloride with linear isoprenoids
Veselovskii, V. V.; Dragan, V. A.; Moiseenkov, A. M.

CORPORATE SOURCE: Inst. Org. Khim. im. Zelinskogo, Moscow, USSR

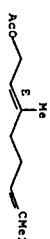
IZVESTIYA AKADEMII NAUK SSSR, SERIYA KHIMICHESKAYA (1987), (12), 2787-90

CODEN: IASRA6; ISSN: 0002-3353
DOCUMENT TYPE: Journal

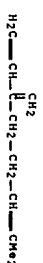
LANGUAGE: Russian
OTHER SOURCE(S): CASREACT 109:93347
ED Entered STN: 17 Sep 1988
AB Treating RCH=CMe₂ [R = CH₂CH₂C(CH₂)CH:CH₂, trans- and cis-CH₂CH₂CMe:CHCH₂OMe, CH₂CH₂CMe:CHCH₂CH₂CMe:CHCO₂Et] with PhSOCl in Me₂CHNO₂ containing ZnCl₂ gave 50-65% PhSOCH₂CHMe:CH₂ (I) which underwent a sulfoxide-sulfonate rearrangement in the presence of P(OMe)₃-MeOH to give 85-90% E-RCH=CMeCH₂OMe. Grignard reaction of I (R = CH₂CH₂C(CH₂)CH:CH₂) with Me₂C=CHCH₂Cl in the presence of CuI-TfH gave 34% of a 4:1 E/Z mixture of Me₂C=CHCH₂CH₂CMe:CHCH₂CH₂C(CH₂)CH:CH₂.

IT 105-87-3 123-35-3 141-12-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(regioselective ene reaction of, with benzenesulfinyl chloride)
RN 105-87-3 HCAPLUS
CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



RN 123-35-3 HCAPLUS
CN 1,6-Octadiene, 7-methyl-3-methylene- (CA INDEX NAME)



RN 141-12-8 HCAPLUS
CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2Z) - (CA INDEX NAME)

Double bond geometry as shown.



CC 30-15 (Terpenes and Terpenoids)
IT 105-87-3 123-35-3 141-12-8
19954-66-6

RL: RCT (Reactant); RACT (Reactant or reagent)
(regioselective ene reaction of, with benzenesulfinyl chloride)

L74 ANSWER 44 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1988:51061 HCAPLUS Full-text
DOCUMENT NUMBER: 109:11061
TITLE: Regioselective ene reaction of benzenesulfinyl chloride with linear isoprenoids

AUTHOR(S):

Moiseenko, A. M.; Dragan, V. A.; Koptenkova, V. A.; Veselovskii, V. V.

CORPORATE SOURCE: N. D. Zelinskii Inst. Org. Chem., Moscow, USSR

SOURCE: Synthesis (1987), (9), 814-15

CODEN: SYNTHF; ISSN: 0039-7881

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 109:11061

ED Entered STN: 01 Oct 1988

AB The Lewis acid (e.g., ZnCl₂) catalyzed ene reaction of PhSOCl with myrcene, geranyl and neryl acetates, as well as Et (E,E)-farnesate proceeds smoothly and chemoselectively by exclusive attack at the terminal trisubstituted C:C bond to give allylic sulfoxides.

IT 105-87-3, Geranyl acetate 123-35-3, Myrcene

141-12-8, Neryl acetate

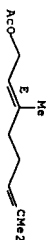
RL: RCT (Reactant); RACT (Reactant or reagent)

(ene reaction of, with benzenesulfinyl chloride)

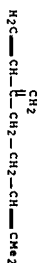
RN 105-87-3 HCAPLUS

CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2E) - (CA INDEX NAME)

Double bond geometry as shown.



RN 123-35-3 HCAPLUS
CN 1,6-Octadiene, 7-methyl-3-methylene- (CA INDEX NAME)



RN 141-12-8 HCAPLUS
CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2Z) - (CA INDEX NAME)

Double bond geometry as shown.



CC 30-10 (Terpenes and Terpenoids)
IT 105-87-3, Geranyl acetate 123-35-3, Myrcene
141-12-8, Neryl acetate 19954-66-6

RL: RCT (Reactant); RACT (Reactant or reagent)
(ene reaction of, with benzenesulfinyl chloride)

L74 ANSWER 45 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1986:481183 HCAPLUS Full-text
DOCUMENT NUMBER: 105:81183
TITLE: Tertiary, optionally halogenated allylic esters

INVENTOR(S):

Mulhauser, Michel

PATENT ASSIGNEE(S):

Rhone-Poulenc Sante, Ft.

SOURCE: Eur. Pat. Appl., 16 pp.

CODEN: EPXXDW

PATENT INFORMATION: Patent

FAMILY ACC. NUM. COUNT: 2

LANGUAGE: French

PATENT NO.:

KIND:

DATE:

APPLICATION NO.:

DATE:

EP 179685

AI 19860430

EP 1985-401819

1985

0919

EP 179685

AI 19860430

EP 1985-401819

1985

0919

EP 179685

AI 19860430

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AI 19860430

EP 1985-401819

1985

0919

EP 179685

AI 19860430

EP 1985-401819

1985

0919

EP 179685

AI 19860430

EP 1985-401819

AB A method is described of manufacturing a tertiary, optionally halogenated allylic ester by the reaction of an alkali metal salt of a carboxylic acid with a primary and/or tertiary allylic halide [prepared by hydrohalogenation of an optionally halogenated polyene containing 2 conjugated double bonds and, optionally, 21 more double bond].

The hydronlogenation catalyst is composed of a Cu(II) salt (e.g., CuI or CuCl₂), an ammonium salt (e.g., tetraalkylammonium halide or trialkylamine hydrochloride) or a phosphonium salt (e.g., tetralkyl phosphonium halide). The starting polyene is chosen from myrcene, β -farnesene, β -sperylene, phytatriene and phytasterene. Thus, in a reactor under Ar were combined 330 mL CH₂Cl₂, Et₃N-HCl 3.33, CuI 2.4, and myrcene 164.4 g. The reaction mixture was cooled to -5° and 43 g HCl was added. After the hydrochlorination step, the solution was added to another reactor, under Ar, containing anhydrous NaOAc, 145, CuI 2.4, and Et₃N-HCl 3.3 g. CuI 2.4 g was added and the solution was mixed 18 h at 20°. The reaction mixture was cooled and an intensely blue aqueous phase and a clear brown organic phase were obtained. After decanting, the organic phase was washed with 300 mL aqueous 100 g/L NH₄Cl solution, 2 times with 200 mL H₂O and dried with K₂CO₃. After filtration and solvent evaporation, an oil 237.1 g was obtained, containing 93% linallyl acetate. The yield from myrcene was 84.5%. The selectivity for linallyl acetate, expressed as the ratio of linallyl acetate to the sum of linallyl acetate, geranyl acetate, and neryl acetate, was 97%.

IT	127-09-3	RL: RCT (Reactant); RACT (Reactant or reagent)
		(acetoxylation by, of hydrohalogenated polyenes)
RN	127-09-3	HCAPLUS
CN		Acetic acid, sodium salt (1:1) (CA INDEX NAME)

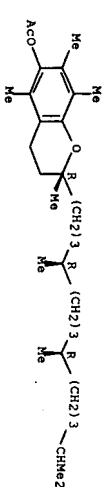
$$\text{HO}-\overset{\text{O}}{\underset{\text{CH}_3}{\text{C}}}-\text{Na}$$

IT	123-35-3	RL: RCT (Reactant); RACT (Reactant or reagent) (hydrohalogenation of, copper halide-quaternary ammonium salt or phosphonium salt-catalyzed)
RN	123-35-3	HCAPLUS
CN	1,6-Octadecene, 7-methyl-3-methylene- (CA INDEX NAME)	

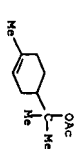
$$\text{H}_2\text{C}=\text{CH}-\underset{\text{CH}_2}{\overset{\text{CH}_2}{\text{C}}}-\text{CH}_2-\text{CH}=\text{CH}_2$$

IT	58-95-7p	RL: PREP (Preparation)
		(manufacture of, by hydrogenation)
RM	58-95-7	HCAPLUS
CN	2H-1-benzopyran-3-ol, 3',4'-dihydro-2',5',7'-octamethyl-2'-(14R,8R)-4',8,12-trimethyl-1'-acetyl-, 6-acetate, (2R) - (CA INDEX NAME)	
	Absolute stereochemistry.	

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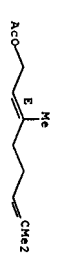


IT	80-26-2P 105-87-3P 115-95-7P
	141-12-8P
RI:	PREP (preparation)
	(manufacture of, copper chloride-triethylamine hydrochloride-catalyzed)
RN	80-26-2 HCAEUS
CN	3-Cyclohexene-1-methanol, $\alpha,\alpha,4$ -trimethyl-, 1-acetate
	(CA INDEX NAME)

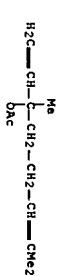


RN	HCAPLUS	(CA INDEX
CN	105-87-3	2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2E)- (CA INDEX NAME)

Double bond geometry as shown

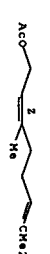


RN	115-95-7	HCAPLUS
CN	1,6-Octadien-3-ol, 3,7-dimethyl-, 3-acetate	(CA INDEX NAME)



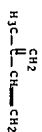
RN	141-12-8	HCAPIUS	
CN	2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2Z)-	(CA INDEX NAME)	

Double bond geometry as shown

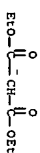


Page 104

IT 78-79-5, reactions
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (addition reaction of, with malonic acid derivs.)
 CN 78-79-5 HCAPLUS
 CN 1,3-Butadiene, 2-methyl- (CA INDEX NAME)

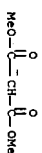


IT 996-82-7 18424-76-5
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (allylation of, in presence of palladium)
 CN 996-82-7 HCAPLUS
 CN Propenedioic acid, 1,3-diethyl ester, ion(1-), sodium (1:1) (CA INDEX NAME)



● Na⁺

RN 18424-76-5 HCAPLUS
 CN Propenedioic acid, dimethyl ester, ion(1-), sodium (1:1) (CA INDEX NAME)



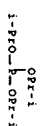
● Na⁺

IT 101-02-0 116-17-6
 RL: CAT (Catalyst use); USES (Uses)
 (catalysts, containing palladium, for substitution of carbanions by allylic derivs.)
 CN 101-02-0 HCAPLUS
 CN Phosphorous acid, triphenyl ester (CA INDEX NAME)

OPH

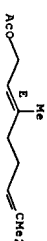


RN 116-17-6 HCAPLUS
 CN Phosphorous acid, tris(1-methylethyl) ester (CA INDEX NAME)

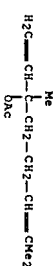


IT 105-87-3 115-95-7 141-12-8
 1191-16-8
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (substitution by, of carbanions in presence of palladium)
 CN 105-87-3 HCAPLUS
 CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2E) - (CA INDEX NAME)

Double bond geometry as shown.



RN 115-95-7 HCAPLUS
 CN 1,6-Octadien-3-ol, 3,7-dimethyl-, 3-acetate (CA INDEX NAME)



RN 141-12-8 HCAPLUS
 CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2Z) - (CA INDEX NAME)

Double bond geometry as shown.



RN 1191-16-8 HCAPLUS
 CN 2-Buten-1-ol, 3-methyl-, 1-acetate (CA INDEX NAME)

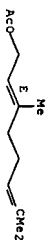


CC 30-10 (Terpenes and Terpenoids)
 Section cross-reference(s): 22, 29
 IT 78-79-5, reactions
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (addition reaction of, with malonic acid derivs.)
 IT 996-82-7 18424-76-5 18852-51-2 19232-39-4
 20334-42-3 24163-38-0 75850-40-7 99372-01-7 99372-24-4
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (allylation of, in presence of palladium)
 IT 101-02-0 116-17-6 122-92-1 603-35-0, uses

Prepared via coupling of the π -allylnickel halide complex derived from $\text{Me}_2\text{C}(\text{CH})_2\text{Br}$ with $\text{BrCH}_2\text{CMe}(\text{CH})_2\text{CH}_2\text{C}(\text{CH}_2)_2\text{CH}_2$ (II) or similar reaction of the π -allylnickel complex derived from II with OBr , resp.

IT 105-87-3 141-12-8
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (Grignard reaction of, with (bromomethyl)furan)
 RN 105-87-3 HCAPLUS
 CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2E)- (CA INDEX NAME)

Double bond geometry as shown.

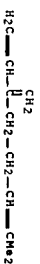


RN 141-12-8 HCAPLUS
 CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2Z)- (CA INDEX NAME)

Double bond geometry as shown.



IT 123-35-3
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (oxidation of)
 RN 123-35-3 HCAPLUS
 CN 1,6-Octadiene, 7-methyl-3-methylene- (CA INDEX NAME)



CC 30-20 (Terpenes and Terpenoids)
 IT 105-87-3 141-12-8
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (Grignard reaction of, with (bromomethyl)furan)
 IT 123-35-3
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (oxidation of)

L74 ANSWER 50 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1983:454028 HCAPLUS Full-text
 DOCUMENT NUMBER: 99:54028
 TITLE: Allyl chlorides
 PATENT ASSIGNEE(S): Nissan Chemical Industries, Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.
 CODEN: JKKXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

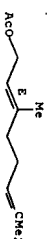
PATENT NO. KIND DATE APPLICATION NO. DATE

JP 58052231 A 19830328 JP 1981-149226 1981
 JP 58052231 A 19830328 JP 1981-149226 0921
 PRIORITY APPL. INFO.: JP 1981-149226 1981
 <--> 0921

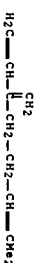
ED Entered STN: 12 May 1984
 AB $\text{RCH}_2\text{CH}(\text{CMe}(\text{CH}_2)_2\text{CH}_2)_2$ (R = terpenyl group) (I) were prepared by reaction of $\text{RCH}_2\text{CH}(\text{CMe}(\text{CH}_2)_2\text{CH}_2)_2$ (R1 = H, Cl, OH, $\text{O}_2\text{SC}_6\text{H}_4$ -p, $\text{O}_2\text{SC}_6\text{H}_4$ -m, $\text{O}_2\text{SC}_6\text{H}_4$ -p, $\text{O}_2\text{SC}_6\text{H}_4$ -m) with trichloroisocyanuric acid. Thus, 19.0 g trichloroisocyanuric acid was added to 39.20 g geranyl acetate in hexane over 30 min, the resulting mixture kept at -5 to 0° for 1 h, and more trichloroisocyanuric acid added at the same temperature until no more unreacted geranyl acetate was detected by gas chromatog. to give 43.53 g I (R = $\text{AcOCH}_2\text{CH}(\text{CMe}(\text{CH}_2)_2\text{CH}_2)_2$).

IT 105-87-3 123-35-3 141-12-8
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (chlorination of, by trichloroisocyanuric acid)
 RN 105-87-3 HCAPLUS
 CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



RN 123-35-3 HCAPLUS
 CN 1,6-Octadiene, 7-methyl-3-methylene- (CA INDEX NAME)



RN 141-12-8 HCAPLUS
 CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2Z)- (CA INDEX NAME)

Double bond geometry as shown.



IC C07C021-04; C07C017-10; C07C021-215; C07C029-62; C07C033-42;
 C07C041-22; C07C043-176; C07C067-287; C07C069-62; C07D311-72
 CC 30-10 (Terpenes and Terpenoids)
 IT 105-87-3 106-25-2 123-35-3 141-12-8
 29548-30-9 52188-73-5 86547-22-0
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (chlorination of, by trichloroisocyanuric acid)

L74 ANSWER 51 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1983:53189 HCAPLUS Full-text

0214

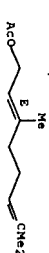
$$\text{H}_3\text{C}-\overset{\text{CH}_2}{\underset{\text{CH}_2}{\text{C}}}-\text{CH}-\text{CH}_2$$

RN	108-05-4	HCAPLUS
CN	Acetic acid ethenyl ester	(CA INDEX NAME)

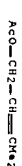
$$\text{AcO}-\text{CH}=\text{CH}_2$$

IT	105-87-3P	1,1,12-8b,11,9,16-8P	
	RL:	SPN (Synthetic preparation); PREP (Preparation)	
		(Preparation of)	
RN	105-87-3	HCAPIUS	
CN	2,6-octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2Z)-	(CA INDEX	
	(NAME)		

Double bond geometry as shown.



CA INDEX NAME	HCAPLUS	RN
1-acetate, 1-methyl-, 3-methyl-, 2-buten-1-ol, CN	1191-16-8	RN
AcO-CH ₂ -CH=CH ₂		



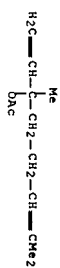
IC COTC67-04
 23-17 (Aliphatic Compounds)
 Section cross-reference(s): 24, 25, 30
 78-79-5, reactions 106-98-9, reactions 106-99-0,
 reactions 108-05-4, reactions 513-33-9 542-92-7,
 reactions 563-65-2 590-18-1 624-66-6
 IT RLT RCT (Reactant); RACR (Reactant or reagent)
 105-97-2P 111-12-8P 542-10-9P 625-16-1P
 628-08-0P 637-27-4P 119-16-8P 2929-48-1P
 RLT: SPN (Synthetic Preparation); PREP (Preparation)
 (preparation of)

1774 ANSWER 52 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STM
ACCESSION NUMBER: 1982;581684 HCAPLUS Full-text
DOCUMENT NUMBER: 97;181684
TITLE: Syntheses by sulfones. XXIII. Selectivity of
the synthesis of allylic sulfones
Julia, Marc; Nel, Maurice; Rightini, Anne;
Uguen, Daniel
CORPORATE SOURCE: Lab. Chim., Ec. Natl. Supér., Paris, 75231,
Fr.
SOURCE: Journal of Organometallic Chemistry (1982), 235(1), 113-20
CODEN: JORCAI; ISSN: 0022-328X

DOCUMENT TYPE: Journal
LANGUAGE: French
OTHER SOURCE(S): CASREACT 97.181684
ED Entered STM: 12 May 1984
AB Pd complexes catalyzed the reaction of conjugated dienes with arenasulfonic acids or of allylic acetates with N₂ arenasulfonates. For example, treatment of isoprene with p-toluenesulfonic acid in the presence of (π-allyl)palladium chloride (I) or bis(dibenzylacetone)palladium and ligands PPh₃, P(C₆H₄Me-o-3), P(C₆H₄Me-3), P(C₆H₄Me-2), or p-Ph₂CH₂CH₂PhPPh₃ gave mainly Me₂C(SO₂CH₂Me)-p-CH=CH₂, along with small amounts of Me₂C:CHCH₂SO₂CH₂Me-p and other minor products. Treatment of Me₂C:CH(CH₂)(2CMe(OAc))CH=CH₂ with Na p-toluenesulfonate in the presence of I and PPh₃ gave 86% Me₂C:CH(CH₂)(2CMe(SO₂CH₂Me)-p)CH=CH₂, 9% E- and 5% Z-Me₂C:CH(CH₂)(2CMe:CHSO₂CH₂Me)-p. Tertiary sulfones are favored under mild reaction conditions. The ligands also influence the reactivity. Arenasulfonic acids catalyzed the isomerization of secondary or tertiary allylic sulfones to primary sulfones.
IT 105-87-3-115-95-7-143-12-6
RL: RCT (Reactant) / RCT (Reactant or reagent)

CC(C)C/C=C/COC

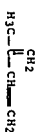
RN	115-95-7	HCAPLUS
CN	1,6-Octadien-3-ol, 3,7-dimethyl-, 3-acetate	(CA INDEX NAME)



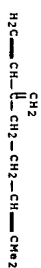
RN	141-12-8	HCAPLUS	
CN	2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2Z)-	(CA INDEX NAME)	

CC(=C)C(C)C/C=C/C#CCOC

IT	78-79-5, reactions 123-35-3
	RL: RCT (Reactant); RACT (Reactant or reagent)
	(reaction of, with toluenesulfonic acid, catalytic)
RN	78-79-5 HCAPLUS
CN	1,3-Butadiene, 2-methyl- (CA INDEX NAME)



RN	123-35-3	HCAPLUS
CN	1,6-Octadiene, 7-methyl-3-methylene-	(CA INDEX NAME)



CC	23-17 (Aliphatic Compounds)
	Section cross-reference(s): 22, 25
IT	105-87-3 115-95-7 141-12-8

RL: RCT (Reactant); RA_{CT} (Reactant or reagent)

174 ANSWER 53 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1981:495775 HCAPLUS Full-text
DOCUMENT NUMBER: 95:95775
TITLE: Use of 1,3,5,5-tetramethyl-2-2

INVENTOR(S) :

PATENT ASSIGNEE(S): International Flavors and Fragrances Inc., USA
SOURCE: U.S., 21 pp. Cont.-in-part of U.S. 4,195,099.

DOCUMENT TYPE:

LANGUAGE: English

PATENT INFORMATION:

[illegible]

US 4269862 A 19810526 US 1979-77539

US 4195099 A 19800325 US 1978-95312

US 4195099	A	19800325	US 1978-953128
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US 4203947 A 19800520 US 1979-8925

US 4203947	A	19800520	US 1979-8925
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US 4283576 A 19810811 US 1979-10052

US 4283576	A	19810811	US 1979-100528
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US 4267067 A 19810512 US 1980-17609

US 4267067	A	19810512	US 1980-176093
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US 4289705 A 19810915 US 1980-17605

US 4289705 A 19810915 US 1980-176050

US 4303725 A 19811201 US 1980-17609

US 4303725 A 19811201 US 1980-176092

US 4320771 A 19820323 US 1980-17611

US 4320771 A 19820323 US 1980-176112

PRIORITY APPLN. INFO.: US 1978-95312

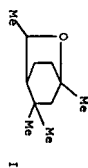
PRIORITY APPLN. INFO.: US 1978-953128 A2 1978

US 1977-85084

US 1977-850845 A3

US 1979-8925

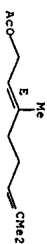
US 1979-0925 A3



AB 1,3,5,5-tetrachloro-2'-oxabicyclo[2,2,2]octane (I) [78474-70-1] is prepared and used to give a fresh or minty flavor to food, tobacco, pharmaceuticals, and other products. Asoprene [78-9-5] to yield 4-acetyl-1,3,3-tetrachloro-1-cyclohexene [15695-36-8]. The latter was reduced with NaBH₄ to give 1,3,3-tetrachloro-1-cyclohexene-6-ethanol [78474-71-2] which was reacted with iso-2-PtOH [67-63-0] and H₂SO₄ to yield I. A eucalyptus oil flavor formulation showed more natural eucalyptus flavor as well as a pleasant citrus nuance and sour effect when I was included at 200 ppm.

IT	105-87-3	141-12-8
	R.I. BIOL (Biological study)	
	(flavoring material containing tetramethylloxacyclooctane and)	
	CN 105-87-3 HCAPUS	
	CN 2,6-octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2E)- (CA INDEX NAME)	

Double bond geometry as shown.

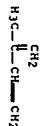


RN	141-12-8	HCAPLUS	
CN	2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2Z)-	(CA INDEX NAME)	

Double bond geometry as shown.



IT 78-79-5, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)



IC	A23L001-226
INCL	426536000
CC	17-2 (Foods

CC 17-2 (Foods

Section cross-reference(s): 62, 63
IT Flavoring materials

IT (tetramethylxylodiolisocitane)	75-07-0, biological studies	78-70-6	80-56-8	87-44-5
92-52-4, biological studies	94-62-2	98-55-5	99-49-0	
99-86-5, 105-87-3	110-89-4, biological studies			
118-71-8	120-65-0	121-33-5	123-11-5, biological studies	
127-91-3	138-86-3	141-12-8	470-82-6	
499-91-0	555-10-2	586-62-9	1329-99-3	4674-50-4
5392-40-5				
14573-74-7	38049-26-2			
RT: BIOL. (Biological study)				

IT 70-79-5, reactions
(flavoring material containing tetramethylxobicyclooctane and
Ru: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with methyl oxide)

L74 ANSWER 54 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1980:568419 HCAPLUS Full-text
DOCUMENT NUMBER: 93:160419
TITLE: Cyclization of polyenes. Part

TITLE:

AUTHOR(S):
CORPORATE SOURCE:
SOURCE:

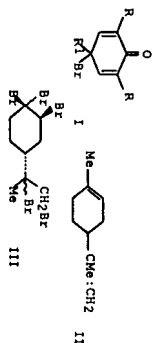
CORPORATE SOURCE:
Dep. Chem., Tohoku Univ., Sendai, 980, Japan
SOURCE:
Journal of the Chemical Society, Perkin
Transactions 1: Organic and Bio-Organic
Chemistry (1972-1999) (1980), (5),
1051-6
CODEN: JCPRB4; ISSN: 0300-922X

DOCUMENT TYPE:

LANGUAGE

OTHER SOURCE(S)

ED Entered STN: 12 May 1984

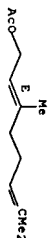


AB Geranyl cyanide reacted with the bromo ketones I (R = R₁ = Br, Cl; R = Br, R₁ = Me) to give a mixture of MeCBrHCHBr(CH₂)₂2CMe:CHCH₂CN, CH₂:CMeHCHBr(CH₂)₂2CMe:CHCH₂CN, and

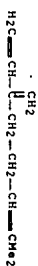
BrCH₂CMe:CH(CH₂)₂CMe:CHCH₂CH with the former predominating in yields of 98, 40, and 45%, resp. This mild selective bromination was extended to a range of polyenes using CTAB and I (R = R₁ = Br). E.g., the polyene II gave 87% III. The di- or tetrabromo products are formed by sequential reactions.

IT 105-87-3 123-35-3
 R₁: RCT (Reactant); RACT (Reactant or reagent)
 (bromination of, by tetrabromocyclohexadecanone, selective)
 RN 105-87-3 HCAPLUS
 CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



RN 123-35-3 HCAPLUS
 CN 1,6-Octadiene, 7-methyl-3-methylene- (CA INDEX NAME)



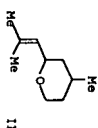
CC 30-10 (Terpenoids)
 Section cross-reference(s): 23, 24
 IT 100-42-5, reactions 105-87-3 110-83-8, reactions
 123-35-3 126-91-0 1189-09-9 4176-77-6 5989-27-5
 6485-40-1 21677-96-3 36237-68-0 42207-88-5
 R₁: RCT (Reactant); RACT (Reactant or reagent)
 (bromination of, by tetrabromocyclohexadecanone, selective)

L74 ANSWER 55 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1980:495409 HCAPLUS Full-text
 DOCUMENT NUMBER: 93:95409

TITLE:
 The reaction of hypochlorous acid with olefins. A convenient synthesis of allylic chlorides

AUTHOR(S):
 Hegde, Shridhar G.; Vogel, Martin K.; Sadler, John; Hirano, Tanya; Rockwell, Ned; Haynes, Robert; Oliver, Michael; Molinsky, Joseph
 CORP. SOURCE: Dep. Chem., Purdue Univ., West Lafayette, IN, 47907, USA
 SOURCE: Tetrahedron Letters (1980), 21(5), 441-4
 CODEN: TETLEA; ISSN: 0040-4039

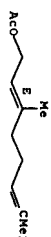
DOCUMENT TYPE: Journal
 LANGUAGE: English
 ED Entered STN: 12 May 1984



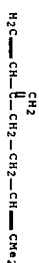
AB HOCl reacts with highly substituted olefins in CH₂Cl₂ to give allylic chlorides. E.g., Me₂C:CH(CH₂)₂CMe:CH(R) (R = CHO, CO₂Me, CH₂OH, CH₂OMe) reacted with HOCl to give 60-80% CH₂:CMeCHCl(CH₂)₂CMe:CH(R) (I). The utility of the reaction is illustrated by preparation of α-monoterpenes and Rose oxide. Thus, sequential treatment of I (R = CHO, CO₂Me, CH₂OH) with Zn-TfP and H₂O gave CH₂:CMe(CH₂)₂CMe:CH(R), and sequential treatment of Me₂C:CH(CH₂)₂CMe(CH₂)₂OR (R = H, Ac) with HOCl, NaOH-ROH, and H₂SO₄ gave, approx. 50% Rose oxide (II).

IT 105-87-3 123-35-3 150-84-5
 R₁: RCT (Reactant); RACT (Reactant or reagent)
 (chlorination of, by hypochlorous acid-methylene chloride)
 RN 105-87-3 HCAPLUS
 CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2E)- (CA INDEX NAME)

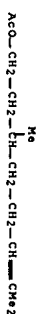
Double bond geometry as shown.



RN 123-35-3 HCAPLUS
 CN 1,6-Octadiene, 7-methyl-3-methylene- (CA INDEX NAME)



RN 150-84-5 HCAPLUS
 CN 6-Octen-1-ol, 3,7-dimethyl-, 1-acetate (CA INDEX NAME)



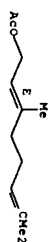
CC 30-10 (Terpenoids)
 Section cross-reference(s): 23
 IT 78-70-6 89-79-2 99-49-0 105-87-3 106-22-9
 106-24-1 106-25-2 123-35-3 141-27-5 150-84-5
 591-49-1 1189-09-9 1195-92-2 4602-84-0 7212-44-4
 13466-78-9 55298-92-5 56695-54-6 74514-15-1 74514-25-3
 R₁: RCT (Reactant); RACT (Reactant or reagent)
 (chlorination of, by hypochlorous acid-methylene chloride)

L74 ANSWER 56 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1979:508091 HCAPLUS Full-text
 DOCUMENT NUMBER: 91:108091

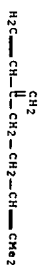
TITLE:
 A facile functionalization of the isopropylidene terminus of isoprenoids. Application to the synthesis of terminal trans allylic alcohols
 AUTHOR(S): Masaki, Yukio; Hashimoto, Kenji; Kaji, Kenji
 CORP. SOURCE: Gifu Coll. Pharm., Gifu, Japan

RN 105-87-3 HCAPLUS
 (Preparation of)
 CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



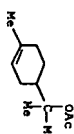
IT 123-35-3
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (Reaction with diethylamine in presence of sodium naphthalenide, diethylgeranylamine from)
 RN 123-35-3 HCAPLUS
 CN 1,6-Octadiene, 7-methyl-3-methylene- (CA INDEX NAME)



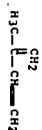
CC 30-10 (Terpenoids)
 IT 105-87-3P 105-90-8P 106-29-6P 109-20-6P 2345-26-8P
 10402-47-8P 56172-46-4P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (Preparation of)
 IT 123-35-3
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (Reaction with diethylamine in presence of sodium naphthalenide, diethylgeranylamine from)

L74 ANSWER 60 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1976:74443 HCAPLUS Full-text
 DOCUMENT NUMBER: 84:74443
 TITLE: Terpenoid alcohols and acetates from the telomerization product of isoprene with its hydrochlorides
 AUTHOR(S): Kaal, T.; Laats, K.
 CORPORATE SOURCE: Inst. Khim., Tallin, USSR
 SOURCE: Vest. NSV Teaduste Akadeemia Toimetised, Keemia, Geoloogia (1975), 24(4), 263-6
 CODEN: EREKAI; ISSN: 0424-6373

DOCUMENT TYPE: Journal
 LANGUAGE: Russian
 ED Entered STN: 12 May 1984
 AB Mixtures of terpene chlorides prepared by telomerization of isoprene with its hydrochlorides were saponified and the unreacted chlorides dehydrochlorinated with alc. KOH to give linalool, MeC(CH=CH)CH(OH)CH=CH2, MeC(CH=CH)CH2CH=CH2, and a mixture of alpha-terpineol and m-menth-6-en-8-ol.
 IT 80-26-2P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (Preparation of)
 RN 80-26-2 HCAPLUS
 CN 3-Cyclohexene-1-methanol, alpha,4-trimethyl-, 1-acetate (CA INDEX NAME)



IT 78-79-5, reactions
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (Telomerization of, with its hydrochlorides, alcs. and acetates from)
 RN 78-79-5 HCAPLUS
 CN 1,3-Butadiene, 2-methyl- (CA INDEX NAME)

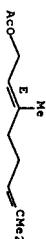


CC 30-10 (Terpenoids)
 IT 80-26-2P 25449-04-1P 58336-04-2P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (Preparation of)
 IT 78-79-5, reactions
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (Telomerization of, with its hydrochlorides, alcs. and acetates from)

L74 ANSWER 61 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1974:13720 HCAPLUS Full-text
 DOCUMENT NUMBER: 80:13720
 TITLE: Reaction of amines with conjugated dienes in the presence of geranyl acetate
 AUTHOR(S): Fujita, T.; Suga, K.; Watanabe, S.
 CORPORATE SOURCE: Fac. Eng., Chiba Univ., Chiba, Japan
 SOURCE: Australian Journal of Chemistry (1974) 1, 27(3), 531-5
 CODEN: AJCHAS; ISSN: 0004-9425

DOCUMENT TYPE: Journal
 LANGUAGE: English
 ED Entered STN: 12 May 1984
 AB Reaction of a conjugated diene with Et2NH using Na naphthalenide in THF gave a mixture of beta,gamma-unsatd. amines. From myrcene, N,N-diethyl-2-ethylidene-6-methylhept-5-enylamine, N,N-diethylheptylamine and N,N-diethylgeranylamine were obtained. Reaction of beta,gamma-unsatd. amines with Ac2O gave a mixture of beta,gamma-unsatd. acetates. From N,N-diethylgeranylamine, a mixture of neryl acetate and geranyl acetate was obtained.
 IT 105-87-3P 101-12-8P 1191-16-8P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (Preparation of)
 RN 105-87-3 HCAPLUS
 CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



RN 141-12-8 HCAPLUS
CN 2,6-Octadiene-1-ol, 3,7-dimethyl-, 1-acetate, (2Z)- (CA INDEX NAME)

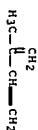
Double bond geometry as shown.



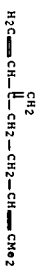
RN 1191-16-8 HCAPLUS
CN 2-Buten-1-ol, 3-methyl-, 1-acetate (CA INDEX NAME)



IT 78-79-5, reactions 123-35-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(With amines, in presence of alkali naphthalenides)
RN 78-79-5 HCAPLUS
CN 1,3-Butadiene, 2-methyl- (CA INDEX NAME)



RN 123-35-3 HCAPLUS
CN 1,6-Octadiene, 7-methyl-3-methylene- (CA INDEX NAME)



CC 23-4 (Aliphatic Compounds)
Section cross-reference(s): 27, 28, 30
IT 105-87-3P 141-12-8P 688-92-6P

24509-88-4P 27973-92-8P 27973-95-1P 36794-55-5P
36794-56-6P 37857-39-9P 37857-40-2P 40137-00-6P
40267-43-4P 40267-47-8P 40267-48-9P 40267-53-6P
51930-65-5P 51930-66-6P 51930-67-7P 51930-68-8P
51930-69-9P 51930-70-2P 51930-72-4P 51930-73-5P
52027-04-0P 59313-90-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(Preparation of)

IT 78-79-5, reactions 123-35-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(With amines, in presence of alkali naphthalenides)

L74 ANSWER 62 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1974:26777 HCAPLUS Full-text
DOCUMENT NUMBER: 80:26777
TITLE: Unsaturated diesters

INVENTOR(S): Ono, Isao; Yanagihara, Tadshisa; Okada,
Hitkazu; Koga, Toshikuni
PATENT ASSIGNEE(S): Toyo Soda Manufg. Co., Ltd.
SOURCE: Jpn. Tokkyo Koho, 4 pp.
CODEN: JAKXAB
Patent
Japanese

DOCUMENT TYPE:
LANGUAGE:
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 4802889	B	19730905	JP 1968-90547	1968 1212

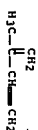
PRIORITY APPLN. INFO.:

JP 1968-90547
1968
1212

Entered STN: 12 May 1984

AB 2-Butene-1,4-diol esters acyclic or cyclic, with alkyl substituents or none, were obtained by reaction of conjugated dienes with carboxylic acids in the presence of Pd salts, transition metal salts, and alkali or alkali metal salts. Thus, 16.3 g butadiene, 100 g AcOH, 0.65 g Pd(OAc)₂, 15.0 g Cu(OAc)₂, and 10.9 g NaOAc was treated at 80° under 15 atm O for 3 hr to give 14.5 g 1,4-diacetoxy-2-butene. Similarly prepared were 1,4-diacetoxy-2-methyl-2-butene, 3,5-dipropionyloxy-1-cyclohexene, and 3,6-diformyloxy-1-cyclohexene.

IT 78-79-5, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(Addition to, of carboxylic acids, catalysts for)
RN 78-79-5 HCAPLUS
CN 1,3-Butadiene, 2-methyl- (CA INDEX NAME)



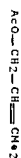
IT 127-09-3
RL: CAT (Catalyst use); USES (Uses)
(Catalysts, with cupric and palladium acetates, for addition of acetic acid to butadienes)
RN 127-09-3 HCAPLUS
CN Acetic acid, sodium salt (1:1) (CA INDEX NAME)



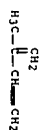
Na

IC C07C
CC 23-17 (Aliphatic Compounds)
Section cross-reference(s): 24
IT Esters, preparation
RL: PREP (Preparation)
(unsatd. di-)

RI: RCT (Reactant); RACT (Reactant or reagent)
(terpenoids from isoprene and)
RN 1191-16-8 HCAPLUS
CN 2-Buten-1-ol, 3-methyl-, 1-acetate (CA INDEX NAME)



IT 78-79-5, reactions
RI: RCT (Reactant); RACT (Reactant or reagent)
(terpenoids from prenyl acetate and)
RN 78-79-5 HCAPLUS
CN 1,3-Butadiene, 2-methyl-, (CA INDEX NAME)

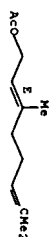


CC 30 (Terpenoids)
IT 80-26-2P 16409-44-2P 24604-60-2P 25905-14-0P
33843-18-4P 33843-20-8P
RI: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT 1191-16-8
RI: RCT (Reactant); RACT (Reactant or reagent)
(terpenoids from isoprene and)
IT 78-79-5, reactions
RI: RCT (Reactant); RACT (Reactant or reagent)
(terpenoids from prenyl acetate and)

174 ANSWER 65 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1970:531138 HCAPLUS Full-text
DOCUMENT NUMBER: 73:131138
TITLE: Complexes of terpenes with transition metals.
III. Dimerization by means of
tetrakis(triphenylphosphine)palladium
Dunne, K.; McQuillan, Francis J.
Dep. Org. Chem., Univ. Newcastle-upon-Tyne,
Newcastle-upon-Tyne, UK
Journal of the Chemical Society [Section] C:
Organic (1970), (16), 2203-6
CODEN: JSOQAX; ISSN: 0022-4952
Journal
LANGUAGE: English

DOCUMENT TYPE:
ED Entered STN: 12 May 1984
AB Tetrakis(triphenylphosphine)palladium dimers, neololyl acetate, and 1-
vinylcyclohexyl acetate to linear dimers, and myrcene to a monocyclic dimeric product.
IT 105-87-3 123-35-3
RI: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with palladium phosphine complexes)
RN 105-87-3 HCAPLUS
CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



RN 123-35-3 HCAPLUS
CN 1,6-Octadiene, 7-methyl-3-methylene- (CA INDEX NAME)

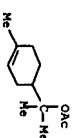


CC 30 (Terpenoids)
IT 105-87-3 123-35-3 2306-78-7,
1,6,10-Dodecatrien-3-ol, 3,7,11-trimethyl-, acetate 6318-49-6
RI: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with palladium phosphine complexes)

174 ANSWER 66 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1970:133026 HCAPLUS Full-text
DOCUMENT NUMBER: 72:133026
TITLE: Terpenyl acetates
INVENTOR(S): Clark, John Colin
SOURCE: A. Boake, Roberts and Co. Ltd.
Brlt., 3 pp.
CODEN: BRXXAA
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 1172516		19691203	GB 1965-51023	1965 1201

ED Entered STN: 12 May 1984
AB The esters of limonol, geraniol, and nerol were prepared from myrcene. Thus, a mixture
of 50 lb 80% myrcene, 250 lb AcOH, and 0.5 lb tert-butylcatechol was stirred in an
inert atmosphere at 110-20° 36 hr to give 10 lb acetate esters, containing 55% geranyl
and nerol acetates, 15% myrcenyl acetates, and 12% α-terpinyl acetate.
IT 80-26-2P 105-87-3P 141-12-0P
RI: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 80-26-2 HCAPLUS
CN 3-Cyclohexene-1-methanol, α,α,4-trimethyl-, 1-acetate
(CA INDEX NAME)



RN 105-87-3 HCAPLUS

IT 78-79-5, reactions 542-92-7 592-57-4
 RL: RCT (Reactant); RACT (Reactant or reagent)
 IT 127-09-3
 RL: CAT (Catalyst use); USES (Uses)
 (catalysts, with cupric and palladium acetates, for addition of acetic acid to butadienes)

L74 ANSWER 63 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1973:418895 HCAPLUS Full-text
 DOCUMENT NUMBER: 79:18895
 TITLE: Terpene alcohols and their acetates and formates

INVENTOR(S): Fukui, Kenichi; Kogitani, Tsutomu; Yamanka, Toru

PATENT ASSIGNEE(S): Takasago Perfumery Co., Ltd.
 SOURCE: Jpn. Tokyo Koho, 2 pp.
 CODEN: JAXXAD

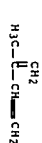
DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 48010766	B	1970407	JP 1969-93950	1969 1125

PRIORITY APPL. INFO.:
 <--
 JP 1969-93950
 1969
1125

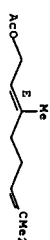
ED Entered STN: 12 May 1984
 AB Terpene alcs. and their acetates and formates were prepared by dimerization of isoprene in liquid CO₂ by catalytic use of 85% H₃PO₄ or 70% H₂SO₄ in the presence of H₂O, AcOH, or HCO₂H. E.g., a mixture of isoprene 34, AcOH 50, 85% H₃PO₄ 24, and CO₂ 100 g was kept 1 hr at 17° to give, after steam distillation, 11.2 g distillate containing geranyl (main), linalyl, myrcenyl, and terpenyl acetates. Geranyl, linalyl, and myrcenyl formates and geraniol, linalol, and myrcenol were also obtained.

IT 78-79-5, (Reaction); RACT (Reactant or reagent)
 RL: RCT (Reactant); RACT (Reactant or reagent)
 RN 78-79-5 HCAPLUS
 CN 1,3-Butadiene, 2-methyl- (CA INDEX NAME)

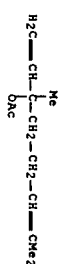


IT 105-87-3P 115-95-7P
 RL: PREP (Preparation)
 (from dimerization of isoprene)
 RN 105-87-3 HCAPLUS
 CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (ZE) - (CA INDEX NAME)

Double bond geometry as shown.



RN 115-95-7 HCAPLUS
 CN 1,6-Octadien-3-ol, 3,7-dimethyl-, 3-acetate (CA INDEX NAME)



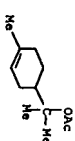
IC COTC: B01J
 CC 30-10 (Terpenoids)
 IT 78-79-5, reactions
 RL: RCT (Reactant); RACT (Reactant or reagent)
 IT 105-87-3P 115-95-7P 118-39-4P 13461-20-6P
 RL: PREP (Preparation)
 (from dimerization of isoprene)

L74 ANSWER 64 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1971:52947 HCAPLUS Full-text
 DOCUMENT NUMBER: 75:12947
 TITLE: Syntheses of terpenoids by telomerization. V. Cationic telomerization of isoprene with prenyl acetate

AUTHOR(S): Takabe, Kunihiko; Katagiri, Takao; Tanaka, Juntao
 CORPORATE SOURCE: Fac. Eng., Shizuoka Univ., Hamamatsu, Japan
 SOURCE: Kogyo Kagaku Zasshi (1971), 74(6), 1162-4
 CODEN: KKGZAT; ISSN: 0368-5462
 DOCUMENT TYPE: Journal
 LANGUAGE: Japanese

ED Entered STN: 12 May 1984
 GI For diagram(s), see printed CA Issue.
 AB A mixture of isoprene 3,4, prenyl acetate (I) 6,4, and EtOAc 6,4 g was mixed dropwise during 10 min with a solution containing 0.9 g BF₃·Et₂O in 1.5 g EtOAc and heated 1 hr at 20°. The structures of the telomers obtained (II-VII) were determined by IR and NMR spectroscopy. The reaction of I in the presence of acidic catalysts was also discussed. Based on the exptl. results, a reaction mechanism was proposed.

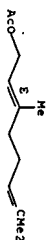
IT 80-26-2P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (Preparation of)
 RN 80-26-2 HCAPLUS
 CN 3-Cyclohexene-1-methanol, α,α,4-trimethyl-, 1-acetate (CA INDEX NAME)



IT 1191-16-8

CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2E)- (CA INDEX NAME)

Double bond geometry as shown.

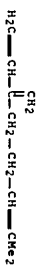


RN 141-12-8 HCAPLUS
CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



IT 123-35-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with acetic acid)
RN 123-35-3 HCAPLUS
CN 1,6-Octadiene, 7-methyl-3-methylene- (CA INDEX NAME)



IC C07C
CC 30 (Terpenoids)
IT 80-26-2P 105-87-3P 141-12-8P
1118-39-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT 123-35-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with acetic acid)

L74 ANSWER 67 OF 67 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1967:76161 HCAPLUS Full-text
DOCUMENT NUMBER: 66:76161
TITLE: Reaction gas chromatography. II.
Dehydrogenation of monoterpene compounds on
platinum-alumina catalyst

AUTHOR(S): Mizrahi, Isaac; Nigam, Ishwar C.
CORPORATE SOURCE: Food Drug Directorate, Ottawa, Can.
JOURNAL OF CHROMATOGRAPHY (1966),
25(2), 230-41
CODEN: JOCRAM; ISSN: 0021-9673

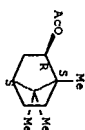
DOCUMENT TYPE: English
LANGUAGE: English
ED Entered STN: 12 May 1984
AB cf. CA 66, 75418P. Dehydrogenation of 42 monoterpenes was investigated using a reactor packed with 5% Pt on Al2O3. Products obtained were analyzed by gas chromatography on 3 instruments using a thermal conductivity detector, and a H flame ionization detector.

Exptl. data correlated with the structures of the parent compds. Mechanisms of dehydrogenations and isomerizations involved were discussed.

IT 76-49-3 105-87-3 115-95-7
123-35-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(dehydrogenation of, chromatog. and)

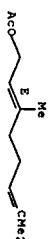
RN 76-49-3 HCAPLUS
CN Bicyclo[2.2.1]heptan-2-ol, 1,7,7-trimethyl-, 2-acetate,
(1R,2S,4R)-tel- (CA INDEX NAME)

Relative stereochemistry.

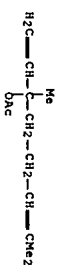


RN 105-87-3 HCAPLUS
CN 2,6-Octadien-1-ol, 3,7-dimethyl-, 1-acetate, (2E)- (CA INDEX NAME)

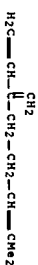
Double bond geometry as shown.



RN 115-95-7 HCAPLUS
CN 1,6-Octadien-3-ol, 3,7-dimethyl-, 3-acetate (CA INDEX NAME)



RN 123-35-3 HCAPLUS
CN 1,6-Octadiene, 7-methyl-3-methylene- (CA INDEX NAME)



CC 30 (Terpenes)
IT 76-49-3 78-70-6 79-92-5 80-56-8, reactions 89-48-5
98-55-5 99-82-1 99-83-2 99-86-5 105-86-2 105-87-3
106-22-9 106-24-1 115-95-7 115-99-1 123-35-3
127-91-3 138-86-3 491-05-4 498-15-7 500-00-5 507-70-0
586-62-9 586-67-4 1134-95-8 1197-07-5 1490-04-6
1632-73-1 3387-41-5 7786-67-6 13877-91-3 29563-98-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(dehydrogenation of, chromatog. and)

-> d his profile

(FILE 'HOME' ENTERED AT 10:23:49 ON 16 MAY 2007)

FILE 'HCAPLUS' ENTERED AT 10:24:09 ON 16 MAY 2007

E US20070055076/PN

L1 1 SEA ABB=ON PLU=ON US20070055076/PN

D ALL

SEL RN

FILE 'REGISTRY' ENTERED AT 10:25:28 ON 16 MAY 2007

L2 35 SEA ABB=ON PLU=ON (100-66-3/BI OR 105-87-3/BI OR

105-90-8/BI OR 105-91-9/BI OR 106-24-1/BI OR 106-25-2/B

1 OR 106-42-3/BI OR 107-92-6/BI OR 108-21-4/BI OR

108-86-3/BI OR 108-90-7/BI OR 108-94-1/BI OR 109-20-6/B

1 OR 1191-16-8/BI OR 123-35-3/BI OR 123-86-4/BI OR

127-08-2/BI OR 127-09-3/BI OR 137-40-6/BI OR 138-86-3/B

1 OR 141-12-8/BI OR 142-96-1/BI OR 157258-67-8/BI OR

19559-59-2/BI OR 3915-83-1/BI OR 503-74-2/BI OR

5392-40-5/BI OR 556-82-1/BI OR 64-19-7/BI OR 78-79-5/BI

OR 78-93-3/BI OR 79-09-4/BI OR 79-31-2/BI OR 80-26-2/B

1 OR 851785-97-2/BI)

L3 19 SEA ABB=ON PLU=ON L2 AND ?ACID?/CNS

D SCAN

L4 1 SEA ABB=ON PLU=ON 123-35-3/RN

D SCAN

D IDE

L5 1 SEA ABB=ON PLU=ON 78-79-5/RN

D SCAN

D IDE

L6 1 SEA ABB=ON PLU=ON 1191-16-8/RN

D SCAN

D CN

D IDE

L7 1 SEA ABB=ON PLU=ON 105-87-3/RN

D SCAN

D IDE

L8 1 SEA ABB=ON PLU=ON 141-12-8/RN

D IDE

L9 11 SEA ABB=ON PLU=ON L2 AND ?ACETATE?/CNS

FILE 'STINGUIDE' ENTERED AT 10:44:21 ON 16 MAY 2007

FILE 'CASREACT' ENTERED AT 10:50:09 ON 16 MAY 2007

L10 1 SEA ABB=ON PLU=ON 123-35-3/RCT(L) (105-87-3/PRO OR

141-12-8/PRO)

D SCAN

L11 2 SEA ABB=ON PLU=ON 78-79-5/RCT(L) (1191-16-8/PRO

D SCAN

E ESTER/CT

E ESTERS/CT

L12 23 SEA ABB=ON PLU=ON 64-19-7/RCT(L) (123-35-3/RCT OR

78-79-5/RCT)

D SCAN

L13 STR 123-35-3

L14 36 SEA SSS SAM L13 (448 REACTIONS)

L15 789 SEA SSS FUL L13 (11229 REACTIONS)

SAV L15 LA0307CRCT/A

E ESTERS/CT

L16 7147 SEA ABB=ON PLU=ON ESTERS+PFT OLD,NT/CT

L17 7 SEA ABB=ON PLU=ON L15 AND L16

D SCAN

D QUE

SN 10/564307 Page 137 of 139 STIC STN SEARCH 5/17/2007

L18 SAV L17 LA0307CRCTA/A
 L19 STR L13
 L20 6 SEA SUB-L15 SSS SAM L18 (28 REACTIONS)
 L21 D SCAN
 L22 88 SEA SUB-L15 SSS FUL L18 (708 REACTIONS)
 L23 SAV L20 LA0307CRCTB/A
 L24 STR L18
 L25 1 SEA SUB-L15 SSS SAM L21 (7 REACTIONS)
 L26 D SCAN
 L27 5 SEA SUB-L15 SSS FUL L21 (16 REACTIONS)
 L28 SAV L23 LA0307CRCTC/A
 L29 STR L21
 L30 1 SEA SUB-L15 SSS SAM L24 (7 REACTIONS)
 L31 D SCAN
 L32 7 SEA SUB-L15 SSS FUL L24 (38 REACTIONS)
 L33 D SCAN
 L34 SAV L26 LA0307CRCTD/A
 L35 STR L27 LA0307CRCTE/A
 L36 34 SEA AB-B-ON PLU-ON (L10 OR L11 OR L12) OR L17 OR L23
 L37 OR L26
 L38 43 SEA AB-B-ON PLU-ON BABLER JAMES?/AU
 L39 3 SEA AB-B-ON PLU-ON L27 AND L28
 L40 SAV L29 LA0307CRCTIN/A
 L41 31 SEA AB-B-ON PLU-ON L27 NOT L29
 L42 FILE 'HCAPIUS' ENTERED AT 12:06:06 ON 16 MAY 2007
 L43 QUE AB-B-ON PLU-ON PY<2004 OR PRY<2004 OR AY<2004 OR
 L44 MY<2004 OR REVIEW/DT
 L45 1 SEA AB-B-ON PLU-ON L1 AND L31
 L46 D SCAN
 L47 FILE 'CASREACT' ENTERED AT 12:07:53 ON 16 MAY 2007
 L48 25 SEA AB-B-ON PLU-ON L30 AND L31
 L49 3 SEA AB-B-ON PLU-ON L29 AND L31
 L50 FILE 'HCAPIUS' ENTERED AT 12:08:48 ON 16 MAY 2007
 L51 D SCAN L1
 L52 619 SEA AB-B-ON PLU-ON L4/RACT
 L53 5537 SEA AB-B-ON PLU-ON L5/RACT
 L54 86 SEA AB-B-ON PLU-ON L6/P
 L55 347 SEA AB-B-ON PLU-ON L7/P
 L56 D 1-2 KWIC
 L57 144 SEA AB-B-ON PLU-ON L8/P
 L58 D KWIC
 L59 D 1-2 L36 KWIC
 L60 0 SEA AB-B-ON PLU-ON L36(L) L37
 L61 12 SEA AB-B-ON PLU-ON L36 AND L37
 L62 0 SEA AB-B-ON PLU-ON L35(L) (L38 OR L39)
 L63 10 SEA AB-B-ON PLU-ON L35 AND (L38 OR L39)
 L64 20 SEA AB-B-ON PLU-ON (L40 OR L41 OR L42 OR L43)
 L65 34845 SEA AB-B-ON PLU-ON L9
 L66 70 SEA AB-B-ON PLU-ON (L35 OR L36) AND L45
 L67 4036 SEA AB-B-ON PLU-ON L9/RACT
 L68 50 SEA AB-B-ON PLU-ON (L35 OR L36) AND L47
 L69 9 SEA AB-B-ON PLU-ON L48 AND L44
 L70 E ESTERS/CT
 L71 QUE AB-B-ON PLU-ON ESTERS+PFT, OLD, NT/CT
 L72 70 SEA AB-B-ON PLU-ON L44 OR L46 OR (L48 OR L49)
 L73 47 SEA AB-B-ON PLU-ON L51 AND L50
 L74 E VITAMINS/CT
 L75 QUE AB-B-ON PLU-ON VITAMINS+PFT, OLD, NT/CT
 L76 E FLAVOR/CT
 L77 E FLAVORS/CT
 L78 E FLAVORING/CT
 L79 QUE AB-B-ON PLU-ON FLAVOR+PFT, OLD, NT/CT

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L55 3 SEA AB-B-ON PLU-ON L51 AND (L53 OR L54)
 L56 D SCAN
 L57 D SCAN L1
 L58 E "DIETARY SUPPLEMENTS"/CT
 L59 QUE AB-B-ON PLU-ON "DIETARY SUPPLEMENTS"+PFT, OLD, NT/CT
 L60 QUE AB-B-ON PLU-ON "FLAVORING MATERIALS"+PFT, OLD, NT/CT
 L61 QUE AB-B-ON PLU-ON "ODOR AND ODOROUS SUBSTANCES"+PFT, O
 L62 LD, NT/CT
 L63 45 SEA AB-B-ON PLU-ON L52 AND L31
 L64 SAV L59 LA0307HCE/A
 L65 43 SEA AB-B-ON PLU-ON L28
 L66 D QUE
 L67 43 SEA AB-B-ON PLU-ON L60 AND L31
 L68 QUE AB-B-ON PLU-ON VITAM? OR ODOR? OR SMELL? OR
 L69 PERFUM? OR SUPPLEMENT? OR FLAVOR?
 L70 4 SEA AB-B-ON PLU-ON L61 AND L62
 L71 4 SEA AB-B-ON PLU-ON L61 AND (L53 OR L56 OR L57 OR L58)
 L72 D QUE
 L73 5 SEA AB-B-ON PLU-ON L51 AND (L53 OR L56 OR L57 OR L58)
 L74 45 SEA AB-B-ON PLU-ON L55 OR L59 OR L65
 L75 45 SEA AB-B-ON PLU-ON L66 AND L31
 L76 SAV L67 LA0307HCE/A
 L77 6 SEA AB-B-ON PLU-ON L63 OR L64
 L78 13 SEA AB-B-ON PLU-ON L61 AND L50
 L79 17 SEA AB-B-ON PLU-ON L68 OR L69
 L80 SAV L70 LA0307HCPIN/A
 L81 D QUE L67
 L82 43 SEA AB-B-ON PLU-ON L67 NOT L70
 L83 D QUE L34
 L84 D QUE L33
 L85 FILE 'CASREACT' ENTERED AT 12:45:36 ON 16 MAY 2007
 L86 D QUE L33
 L87 FILE 'STINGUIDE' ENTERED AT 12:46:03 ON 16 MAY 2007
 L88 FILE 'MEDLINE, BIOSIS, DRUGU, EMBASE' ENTERED AT 12:46:36 ON 16
 L89 MAY 2007
 L90 4 SEA AB-B-ON PLU-ON L28
 L91 D 1-4 TI
 L92 SAV L72 LA0307IN/A
 L93 FILE 'STINGUIDE' ENTERED AT 12:47:53 ON 16 MAY 2007
 L94 D QUE L34
 L95 D QUE L70
 L96 D QUE L72
 L97 FILE 'CASREACT, HCAPIUS, BIOSIS' ENTERED AT 12:49:46 ON 16 MAY
 L98 2007
 L99 19 DUP REM L34 L70 L72 (5 DUPLICATES REMOVED)
 L100 ANSWERS '1-3' FROM FILE CASREACT
 L101 ANSWERS '4-18' FROM FILE HCAPIUS
 L102 ANSWER '19' FROM FILE BIOSIS
 L103 FILE 'CASREACT' ENTERED AT 12:51:20 ON 16 MAY 2007
 L104 FILE 'CASREACT, HCAPIUS, BIOSIS' ENTERED AT 12:57:01 ON 16 MAY
 L105 2007
 L106 D L73 1-19 IBIB ABS
 L107 FILE 'CASREACT' ENTERED AT 12:57:02 ON 16 MAY 2007

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FILE 'REGISTRY' ENTERED AT 12:57:42 ON 16 MAY 2007

D L4 IDE
D L5 IDE
D L6 IDE
D L7 IDE
D L8 IDE

FILE 'STINGUIDE' ENTERED AT 12:59:34 ON 16 MAY 2007

D QUE STAT L33
D QUE STAT L71

L74 FILE 'CASREACT, HCAPLUS' ENTERED AT 13:00:44 ON 16 MAY 2007
67 DUP REM L33 L71 (1 DUPLICATE REMOVED)

ANSWERS '1-25' FROM FILE CASREACT
ANSWERS '26-67' FROM FILE HCAPLUS
D L74 1-25 IBIB ABS FHIT
D L74 26-67 IBIB ED ABS HITSTR HITIND